Anthracene, 2-ethyl-

Other names: 2-Ethylanthracene
Inchi: InChI=1S/C16H14/c1-2-12-7-8-15-10-13-5-3-4-6-14(13)11-16(15)9-12/h3-11H,2H2,1H3
InchiKey: ZXAGXLDEMUNQSH-UHFFFAOYSA-N
Formula: C16H14
SMILES: CCc1ccc2cc3ccccc3cc2c1
Mol. weight [g/mol]: 206.28
CAS: 52251-71-5

Physical Properties

Property code	Value	Unit	Source
gf	390.29	kJ/mol	Joback Method
hf	222.16	kJ/mol	Joback Method
hfus	24.50	kJ/mol	Joback Method
hsub	107.60 ± 0.60	kJ/mol	NIST Webbook
hvap	91.40 ± 1.10	kJ/mol	NIST Webbook
log10ws	-6.89		Aqueous Solubility Prediction Method
logp	4.555		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	337.28		NIST Webbook
rinpol	337.28		NIST Webbook
tb	640.08	K	Joback Method
tc	883.76	K	Joback Method
tf	427.60	K	Thermochemistry of some alkylsubstituted anthracenes
vc	0.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.53	J/mol×K	640.08	Joback Method
cpg	446.38	J/mol×K	680.69	Joback Method
cpg	461.00	J/mol×K	721.31	Joback Method

cpg	474.53	J/mol×K	761.92	Joback Method
cpg	487.10	J/mol×K	802.53	Joback Method
cpg	498.83	J/mol×K	843.15	Joback Method
cpg	509.85	J/mol×K	883.76	Joback Method
dvisc	0.0014025	Pa×s	386.94	Joback Method
dvisc	0.0010464	Pa×s	429.13	Joback Method
dvisc	0.0008227	Pa×s	471.32	Joback Method
dvisc	0.0006730	Pa×s	513.51	Joback Method
dvisc	0.0005675	Pa×s	555.70	Joback Method
dvisc	0.0004902	Pa×s	597.89	Joback Method
dvisc	0.0004317	Pa×s	640.08	Joback Method
hsubt	104.90 ± 0.60	kJ/mol	351.00	NIST Webbook
pvap	1.92e-04	kPa	330.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.25e-06	kPa	300.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.36e-05	kPa	310.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	7.01e-05	kPa	320.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.77e-06	kPa	298.15	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	4.90e-04	kPa	340.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.17e-03	kPa	350.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.62e-03	kPa	360.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	5.54e-03	kPa	370.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.01	kPa	380.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.02	kPa	390.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.04	kPa	400.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	0.07	kPa	410.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.12	kPa	420.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.20	kPa	430.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.31	kPa	440.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.49	kPa	450.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	0.74	kPa	460.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	1.09	kPa	470.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

pvap	1.58	kPa	480.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	2.23	kPa	490.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	3.09	kPa	500.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons
pvap	4.22	kPa	510.00	Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Thermochemistry of some alkylsubstituted anthracenes:	https://www.doi.org/10.1016/j.jct.2005.06.001
Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:	https://www.doi.org/10.1021/je800300x
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52251715&Units=SI

Legend

cpg:	Ideal gas heat capacity

dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume