ANTHRACENE, 9-ETHYL-

Other names: 9-Ethylanthracene
Inchi: InChI=1S/C16H14/c1-2-14-15-9-5-3-7-12(15)11-13-8-4-6-10-16(13)14/h3-11H,2H2,1H3
InchiKey: ZFBBPVJBVIJQCE-UHFFFAOYSA-N
Formula: C16H14
SMILES: CCc1c2ccccc2cc2ccccc12
Mol. weight [g/mol]: 206.29
CAS: 605-83-4

Physical Properties

Property code	Value	Unit	Source
af	0.5001		Cheméo Relay (1.0)
hf	167.40	kJ/mol	Cheméo Relay (1.0)
hfus	24.50	kJ/mol	Joback Method
hvap	87.57	kJ/mol	Cheméo Relay (1.0)
ie	7.32	eV	Cheméo Relay (1.0)
log10ws	-6.26		Cheméo Relay (1.0)
logp	4.555		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	353.52		NIST Webbook
tb	634.25	K	Cheméo Relay (1.0)
tc	885.89	K	Cheméo Relay (1.0)
tf	357.54	K	Cheméo Relay (1.0)
vc	0.647	m3/kmol	Cheméo Relay (1.0)

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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.29338e+01
Coeff. B	-4.38417e+03
Coeff. C	-1.21066e+02
Temperature range (K), min.	467.74
Temperature range (K), max.	696.24

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C605834&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor

cpg: Ideal gas heat capacity

dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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