Phenanthrene, 2-ethyl-

Other names: 2-Ethyl-phenanthrene
Inchi: InChI=1S/C16H14/c1-2-12-7-10-16-14(11-12)9-8-13-5-3-4-6-15(13)16/h3-11H,2H2,1H3
InchiKey: UMAHMIHRNVICDZ-UHFFFAOYSA-N
Formula: C16H14
SMILES: CCc1ccc2c(ccc3ccccc32)c1
Mol. weight [g/mol]: 206.28
CAS: 3674-74-6

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
hvap	58.09	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	4.555		Crippen Method
mcvol	173.620	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	337.14		NIST Webbook
rinpol	337.00		NIST Webbook
rinpol	335.44		NIST Webbook
rinpol	336.46		NIST Webbook
rinpol	337.50		NIST Webbook
rinpol	335.40		NIST Webbook
rinpol	336.60		NIST Webbook
rinpol	337.50		NIST Webbook
rinpol	1851.00		NIST Webbook
rinpol	335.53		NIST Webbook
rinpol	1851.00		NIST Webbook
tb	640.08	K	Joback Method
tc	883.76	K	Joback Method
tf	386.94	K	Joback Method
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

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3674746&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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume