1-ETHYL-2-METHYLPHENANTHRENE

Inchi: InChI=1S/C17H16/c1-3-14-12(2)8-10-17-15-7-5-4-6-13(15)9-11-16(14)17/h4-11H,3H2,1-
InchiKey: VLNXCHLISOFWQB-UHFFFAOYSA-N
Formula: C17H16
SMILES: CCc1c(C)ccc2c1ccc1ccccc12
Mol. weight [g/mol]: 220.32

Physical Properties

Property code	Value	Unit	Source
af	0.5313		Cheméo Relay (1.0)
gf	389.08	kJ/mol	Joback Method
hf	127.00	kJ/mol	Cheméo Relay (1.0)
hfus	26.70	kJ/mol	Joback Method
hvap	92.02	kJ/mol	Cheméo Relay (1.0)
ie	7.69	eV	Cheméo Relay (1.0)
log10ws	-6.43		Cheméo Relay (1.0)
logp	4.864		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	652.32	K	Cheméo Relay (1.0)
tc	892.89	K	Cheméo Relay (1.0)
tf	361.99	K	Cheméo Relay (1.0)
vc	0.700	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.42	J/mol×K	667.94	Joback Method
cpg	496.53	J/mol×K	707.84	Joback Method
cpg	511.50	J/mol×K	747.74	Joback Method
cpg	525.45	J/mol×K	787.64	Joback Method
cpg	538.48	J/mol×K	827.54	Joback Method
cpg	550.72	J/mol×K	867.44	Joback Method
cpg	562.29	J/mol×K	907.34	Joback Method
dvisc	0.0012598	Pa×s	410.73	Joback Method

dvisc	0.0009568	Pa×s	453.60	Joback Method
dvisc	0.0007620	Pa×s	496.47	Joback Method
dvisc	0.0006292	Pa×s	539.34	Joback Method
dvisc	0.0005345	Pa×s	582.20	Joback Method
dvisc	0.0004643	Pa×s	625.07	Joback Method
dvisc	0.0004106	Pa×s	667.94	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C61983537&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

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume