

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]:	220.31
CAS:	61983-53-7

Physical Properties

Property code	Value	Unit	Source
gf	389.08	kJ/mol	Joback Method
hf	190.05	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	60.98	kJ/mol	Joback Method
log10ws	-6.36		Crippen Method
logp	4.864		Crippen Method
mcvol	187.710	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
tb	667.94	K	Joback Method
tc	907.34	K	Joback Method
tf	410.73	K	Joback Method
vc	0.724	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.42	J/molxK	667.94	Joback Method
cpg	496.53	J/molxK	707.84	Joback Method
cpg	511.50	J/molxK	747.74	Joback Method
cpg	525.45	J/molxK	787.64	Joback Method
cpg	538.48	J/molxK	827.54	Joback Method
cpg	550.72	J/molxK	867.44	Joback Method
cpg	562.29	J/molxK	907.34	Joback Method
dvisc	0.0012598	Paxs	410.73	Joback Method
dvisc	0.0009568	Paxs	453.60	Joback Method

dvisc	0.0007620	Paxs	496.47	Joback Method
dvisc	0.0006292	Paxs	539.34	Joback Method
dvisc	0.0005345	Paxs	582.20	Joback Method
dvisc	0.0004643	Paxs	625.07	Joback Method
dvisc	0.0004106	Paxs	667.94	Joback Method

Sources

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=C61983537&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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