3-Acetylphenanthrene

Other names: Ethanone, 1-(3-phenanthrenyl)-
Ketone, methyl 3-phenanthryl
methyl 3-phenanthryl ketone
Inchi: InChI=1S/C16H12O/c1-11(17)14-9-8-13-7-6-12-4-2-3-5-15(12)16(13)10-14/h2-10H,1H3
InchiKey: JKVNPRNAHRHQDD-UHFFFAOYSA-N
Formula: C16H12O
SMILES: CC(=O)c1ccc2ccc3ccccc3c2c1
Mol. weight [g/mol]: 220.27
CAS: 2039-76-1

Physical Properties

Property code	Value	Unit	Source
gf	261.37	kJ/mol	Joback Method
hf	109.58	kJ/mol	Joback Method
hfus	26.10	kJ/mol	Joback Method
hvap	64.84	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	4.196		Crippen Method
mcvol	175.190	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	693.95	K	Joback Method
tc	943.48	K	Joback Method
tf	436.87	K	Joback Method
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.19	J/mol×K	693.95	Joback Method
cpg	459.14	J/mol×K	735.54	Joback Method
cpg	471.99	J/mol×K	777.13	Joback Method
cpg	483.87	J/mol×K	818.71	Joback Method
cpg	494.92	J/mol×K	860.30	Joback Method
cpg	505.26	J/mol×K	901.89	Joback Method

cpg	515.03	J/mol×K	943.48	Joback Method
dvisc	0.0016094	Pa×s	436.87	Joback Method
dvisc	0.0012091	Pa×s	479.72	Joback Method
dvisc	0.0009519	Pa×s	522.56	Joback Method
dvisc	0.0007771	Pa×s	565.41	Joback Method
dvisc	0.0006528	Pa×s	608.26	Joback Method
dvisc	0.0005611	Pa×s	651.10	Joback Method
dvisc	0.0004914	Pa×s	693.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2039761&Units=SI
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

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