Anthracene, 1,2,3,4-tetrahydro-2-ol, acetate

Inchi: InChI=1S/C16H16O2/c1-11(17)18-16-7-6-14-8-12-4-2-3-5-13(12)9-15(14)10-16/h2-5,8-9
InchiKey: RNEGEEQZZDNBKA-UHFFFAOYSA-N
Formula: C16H16O2
SMILES: CC(=O)OC1CCc2cc3ccccc3cc2C1
Mol. weight [g/mol]: 240.30

Physical Properties

Property code	Value	Unit	Source
gf	98.37	kJ/mol	Joback Method
hf	-147.07	kJ/mol	Joback Method
hfus	26.30	kJ/mol	Joback Method
hvap	65.69	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	3.260		Crippen Method
mcvol	189.660	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
rinpol	2035.00		NIST Webbook
tb	708.40	K	Joback Method
tc	948.86	K	Joback Method
tf	440.82	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	523.15	J/mol×K	708.40	Joback Method
cpg	593.97	J/mol×K	908.78	Joback Method
cpg	581.89	J/mol×K	868.71	Joback Method
cpg	568.86	J/mol×K	828.63	Joback Method
cpg	554.79	J/mol×K	788.55	Joback Method
cpg	539.58	J/mol×K	748.48	Joback Method
cpg	605.20	J/mol×K	948.86	Joback Method
dvisc	0.0004343	Pa×s	708.40	Joback Method
dvisc	0.0005014	Pa×s	663.80	Joback Method

dvisc	0.0005911	Pa×s	619.21	Joback Method
dvisc	0.0007148	Pa×s	574.61	Joback Method
dvisc	0.0008925	Pa×s	530.01	Joback Method
dvisc	0.0011607	Pa×s	485.42	Joback Method
dvisc	0.0015921	Pa×s	440.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109232&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume