Anthracene, 1-acetoxy-8,9-dihydroxy-

Inchi: InChI=1S/C16H12O4/c1-9(17)20-13-7-3-5-11-8-10-4-2-6-12(18)14(10)16(19)15(11)13/h2
InchiKey: MFLRKDLLDFHARW-UHFFFAOYSA-N
Formula: C16H12O4
SMILES: CC(=O)Oc1cccc2cc3cccc(O)c3c(O)c12
Mol. weight [g/mol]: 268.26

Physical Properties

Property code	Value	Unit	Source
gf	-152.87	kJ/mol	Joback Method
hf	-377.26	kJ/mol	Joback Method
hfus	38.85	kJ/mol	Joback Method
hvap	93.27	kJ/mol	Joback Method
log10ws	-4.49		Crippen Method
logp	3.329		Crippen Method
mcvol	192.800	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
rinpol	2439.00		NIST Webbook
tb	877.61	K	Joback Method
tc	1134.60	K	Joback Method
tf	682.54	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	556.34	J/mol×K	877.61	Joback Method
cpg	619.73	J/mol×K	1091.76	Joback Method
cpg	605.82	J/mol×K	1048.93	Joback Method
cpg	592.77	J/mol×K	1006.10	Joback Method
cpg	580.34	J/mol×K	963.27	Joback Method
cpg	568.28	J/mol×K	920.44	Joback Method
cpg	634.75	J/mol×K	1134.60	Joback Method
dvisc	0.0000011	Pa×s	877.61	Joback Method
dvisc	0.0000014	Pa×s	845.10	Joback Method

dvisc	0.0000019	Pa×s	812.59	Joback Method
dvisc	0.0000027	Pa×s	780.08	Joback Method
dvisc	0.0000039	Pa×s	747.56	Joback Method
dvisc	0.0000057	Pa×s	715.05	Joback Method
dvisc	0.0000089	Pa×s	682.54	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=U374777&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