

Anthracene, 1,8-diacetoxy-9-hydroxy-

Inchi:	InChI=1S/C18H14O5/c1-10(19)22-14-7-3-5-12-9-13-6-4-8-15(23-11(2)20)17(13)18(21)16
InchiKey:	VBRLBTHTFWJTRA-UHFFFAOYSA-N
Formula:	C18H14O5
SMILES:	CC(=O)Oc1cccc2cc3cccc(OC(C)=O)c3c(O)c12
Mol. weight [g/mol]:	310.30

Physical Properties

Property code	Value	Unit	Source
gf	-224.96	kJ/mol	Joback Method
hf	-497.50	kJ/mol	Joback Method
hfus	40.65	kJ/mol	Joback Method
hvap	94.53	kJ/mol	Joback Method
log10ws	-5.26		Crippen Method
logp	3.549		Crippen Method
mcvol	222.550	ml/mol	McGowan Method
pc	2687.42	kPa	Joback Method
rinpol	2642.00		NIST Webbook
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tb	924.02	K	Joback Method
tc	1169.39	K	Joback Method
tf	678.04	K	Joback Method
vc	0.793	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.74	J/mol×K	924.02	Joback Method
cpg	710.55	J/mol×K	1128.50	Joback Method
cpg	699.70	J/mol×K	1087.60	Joback Method
cpg	688.83	J/mol×K	1046.71	Joback Method
cpg	677.80	J/mol×K	1005.81	Joback Method
cpg	666.48	J/mol×K	964.92	Joback Method
cpg	721.51	J/mol×K	1169.39	Joback Method
dvisc	0.0000123	Pa×s	924.02	Joback Method

dvisc	0.0000154	Pa×s	883.02	Joback Method
dvisc	0.0000198	Pa×s	842.03	Joback Method
dvisc	0.0000261	Pa×s	801.03	Joback Method
dvisc	0.0000355	Pa×s	760.03	Joback Method
dvisc	0.0000499	Pa×s	719.04	Joback Method
dvisc	0.0000731	Pa×s	678.04	Joback Method

Sources

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=U374776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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