trans-Anthracene, 1,2,3,4-tetrahydro-1,2-diol, diacetate

Inchi: InChI=1S/C18H18O4/c1-11(19)21-17-8-7-15-9-13-5-3-4-6-14(13)10-16(15)18(17)22-12(2

InchiKey: PNDAQWCWYKIKQO-ROUUACIJSA-N

Formula: C18H18O4

SMILES: CC(=O)OC1CCc2cc3ccccc3cc2C1OC(C)=O

Mol. weight [g/mol]: 298.33

Physical Properties

Property code	Value	Unit	Source
gf	-126.42	kJ/mol	Joback Method
hf	-453.49	kJ/mol	Joback Method
hfus	35.34	kJ/mol	Joback Method
hvap	78.99	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.322		Crippen Method
mcvol	225.280	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2250.00		NIST Webbook
tb	825.78	K	Joback Method
tc	1059.77	K	Joback Method
tf	531.28	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	678.20	J/mol×K	825.78	Joback Method
cpg	693.10	J/mol×K	864.78	Joback Method
cpg	706.80	J/mol×K	903.78	Joback Method
cpg	719.34	J/mol×K	942.77	Joback Method
cpg	730.79	J/mol×K	981.77	Joback Method
cpg	741.22	J/mol×K	1020.77	Joback Method
cpg	750.68	J/mol×K	1059.77	Joback Method
dvisc	0.0013115	Pa×s	531.28	Joback Method
dvisc	0.0009809	Pa×s	580.36	Joback Method

dvisc	0.0007676	Pa×s	629.45	Joback Method
dvisc	0.0006223	Pa×s	678.53	Joback Method
dvisc	0.0005191	Pa×s	727.61	Joback Method
dvisc	0.0004430	Pa×s	776.70	Joback Method
dvisc	0.0003852	Pa×s	825.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R109727&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

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