1-(4-Hydroxy-3-methoxyphenyl)octane-3,5-diyl diacetate

InChI: InChI=1S/C19H28O6/c1-5-6-16(24-13(2)20)12-17(25-14(3)21)9-7-15-8-10-18(22)19(11-1

InChIKey: AUBPDZJRJKZQEX-UHFFFAOYSA-N

Formula: C19H28O6

SMILES: CCCC(CC(CCc1ccc(O)c(OC)c1)OC(C)=O)OC(C)=O

Mol. weight [g/mol]: 352.42

CAS: 53254-50-5

Physical Properties

Property code	Value	Unit	Source
gf	-520.46	kJ/mol	Joback Method
hf	-1020.12	kJ/mol	Joback Method
hfus	44.12	kJ/mol	Joback Method
hvap	93.79	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.387		Crippen Method
mcvol	281.430	ml/mol	McGowan Method
pc	1618.07	kPa	Joback Method
rinpol	2357.30		NIST Webbook
tb	920.52	K	Joback Method
tc	1136.08	K	Joback Method
tf	591.10	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.46	J/mol×K	920.52	Joback Method
cpg	918.89	J/mol×K	956.45	Joback Method
cpg	932.30	J/mol×K	992.37	Joback Method
cpg	944.75	J/mol×K	1028.30	Joback Method
cpg	956.27	J/mol×K	1064.23	Joback Method
cpg	966.92	J/mol×K	1100.15	Joback Method
cpg	976.74	J/mol×K	1136.08	Joback Method
dvisc	0.0000444	Pa×s	591.10	Joback Method

dvisc	0.0000200	Pa×s	646.00	Joback Method
dvisc	0.0000103	Pa×s	700.91	Joback Method
dvisc	0.0000058	Pa×s	755.81	Joback Method
dvisc	0.0000035	Pa×s	810.71	Joback Method
dvisc	0.0000023	Pa×s	865.62	Joback Method
dvisc	0.0000016	Pa×s	920.52	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=C53254505&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