Propafenone desamino dihydroxy, acetylated

Inchi: InChI=1S/C24H26O8/c1-16(25)29-14-21(32-18(3)27)15-30-24-12-10-20(31-17(2)26)13-2
InchiKey: DBMTXAYWOUZNNZ-UHFFFAOYSA-N
Formula: C24H26O8
SMILES: CC(=O)OCC(COc1ccc(OC(C)=O)cc1C(=O)CCc1ccccc1)OC(C)=O
Mol. weight [g/mol]: 442.46

Physical Properties

Property code	Value	Unit	Source
gf	-581.36	kJ/mol	Joback Method
hf	-1073.05	kJ/mol	Joback Method
hfus	52.84	kJ/mol	Joback Method
hvap	111.13	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	3.301		Crippen Method
mcvol	331.260	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	2950.00		NIST Webbook
rinpol	2950.00		NIST Webbook
tb	1116.56	K	Joback Method
tc	1367.05	K	Joback Method
tf	711.76	K	Joback Method
vc	1.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1073.50	J/mol×K	1116.56	Joback Method
cpg	1079.55	J/mol×K	1158.31	Joback Method
cpg	1083.41	J/mol×K	1200.06	Joback Method
cpg	1085.10	J/mol×K	1241.80	Joback Method
cpg	1084.63	J/mol×K	1283.55	Joback Method
cpg	1082.00	J/mol×K	1325.30	Joback Method
cpg	1077.23	J/mol×K	1367.05	Joback Method
dvisc	0.0001112	Pa×s	711.76	Joback Method

dvisc	0.0000680	Pa×s	779.23	Joback Method
dvisc	0.0000450	Pa×s	846.69	Joback Method
dvisc	0.0000316	Pa×s	914.16	Joback Method
dvisc	0.0000233	Pa×s	981.63	Joback Method
dvisc	0.0000179	Pa×s	1049.09	Joback Method
dvisc	0.0000142	Pa×s	1116.56	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=R582939&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