Propafenone hydroxy - H2O, acetylated

Inchi: InChI=1S/C25H29NO5/c1-4-15-26(19(2)27)16-8-17-30-25-14-12-22(31-20(3)28)18-23(25
InchiKey: BQYXEDZTMYPJBG-PXNMLYILSA-N
Formula: C25H29NO5
SMILES: CCCN(C=CCOc1ccc(OC(C)=O)cc1C(=O)CCc1ccccc1)C(C)=O
Mol. weight [g/mol]: 423.50

Physical Properties

Property code	Value	Unit	Source
gf	-40.58	kJ/mol	Joback Method
hf	-526.64	kJ/mol	Joback Method
hfus	58.21	kJ/mol	Joback Method
hvap	104.18	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.578		Crippen Method
mcvol	337.720	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	3050.00		NIST Webbook
rinpol	3050.00		NIST Webbook
tb	1057.77	K	Joback Method
tc	1296.69	K	Joback Method
tf	671.03	K	Joback Method
vc	1.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1097.69	J/mol×K	1057.77	Joback Method
cpg	1109.92	J/mol×K	1097.59	Joback Method
cpg	1120.85	J/mol×K	1137.41	Joback Method
cpg	1130.59	J/mol×K	1177.23	Joback Method
cpg	1139.21	J/mol×K	1217.05	Joback Method
cpg	1146.81	J/mol×K	1256.87	Joback Method
cpg	1153.47	J/mol×K	1296.69	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=R582964&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
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