Propafenone - H2O, acetylated

Inchi: InChI=1S/C23H27NO3/c1-3-16-24(19(2)25)17-9-18-27-23-13-8-7-12-21(23)22(26)15-14-
InchiKey: ALMQNLWWCFYABA-MFOYZWKCSA-N
Formula: C23H27NO3
SMILES: CCCN(C=CCOc1ccccc1C(=O)CCc1ccccc1)C(C)=O
Mol. weight [g/mol]: 365.47

Physical Properties

Property code	Value	Unit	Source
gf	186.13	kJ/mol	Joback Method
hf	-229.09	kJ/mol	Joback Method
hfus	50.63	kJ/mol	Joback Method
hvap	89.91	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.653		Crippen Method
mcvol	302.100	ml/mol	McGowan Method
pc	1456.79	kPa	Joback Method
rinpol	2930.00		NIST Webbook
tb	930.74	K	Joback Method
tc	1155.87	K	Joback Method
tf	563.81	K	Joback Method
vc	1.135	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.27	J/mol×K	930.74	Joback Method
cpg	958.13	J/mol×K	968.26	Joback Method
cpg	971.86	J/mol×K	1005.78	Joback Method
cpg	984.58	J/mol×K	1043.31	Joback Method
cpg	996.36	J/mol×K	1080.83	Joback Method
cpg	1007.31	J/mol×K	1118.35	Joback Method
cpg	1017.52	J/mol×K	1155.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R582959&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
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