Maprotiline M(HO-ethanediyl), diacetylated

Inchi: InChI=1S/C24H27NO3/c1-16(26)25(3)14-8-13-24-15-22(28-17(2)27)23(18-9-4-6-11-20(1
InchiKey: YBWDEKJGURQSAU-UHFFFAOYSA-N
Formula: C24H27NO3
SMILES: CC(=O)OC1CC2(CCCN(C)C(C)=O)c3ccccc3C1c1ccccc12
Mol. weight [g/mol]: 377.48

Physical Properties

Property code	Value	Unit	Source
gf	237.20	kJ/mol	Joback Method
hf	-225.60	kJ/mol	Joback Method
hfus	47.87	kJ/mol	Joback Method
hvap	90.86	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.012		Crippen Method
mcvol	298.770	ml/mol	McGowan Method
pc	1524.69	kPa	Joback Method
rinpol	2996.00		NIST Webbook
tb	954.95	K	Joback Method
tc	1187.49	K	Joback Method
tf	655.26	K	Joback Method
vc	1.139	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.98	J/mol×K	954.95	Joback Method
cpg	1015.50	J/mol×K	993.71	Joback Method
cpg	1036.33	J/mol×K	1032.46	Joback Method
cpg	1057.75	J/mol×K	1071.22	Joback Method
cpg	1080.02	J/mol×K	1109.98	Joback Method
cpg	1103.42	J/mol×K	1148.74	Joback Method
cpg	1128.21	J/mol×K	1187.49	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=R310997&Units=SI

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