Maprotiline M(Nor-HO), diacetylated

Inchi: InChI=1S/C23H25NO3/c1-15(25)24-13-5-11-23-12-10-18(19-6-3-4-7-21(19)23)20-9-8-17
InchiKey: FRCXBZROBTZGDE-UHFFFAOYSA-N
Formula: C23H25NO3
SMILES: CC(=O)NCCCC12CCC(c3ccccc31)c1ccc(OC(C)=O)cc12
Mol. weight [g/mol]: 363.45

Physical Properties

Property code	Value	Unit	Source
gf	205.47	kJ/mol	Joback Method
hf	-210.15	kJ/mol	Joback Method
hfus	45.90	kJ/mol	Joback Method
hvap	94.00	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.053		Crippen Method
mcvol	284.680	ml/mol	McGowan Method
pc	1690.72	kPa	Joback Method
rinpol	3150.00		NIST Webbook
tb	979.45	K	Joback Method
tc	1217.15	K	Joback Method
tf	680.94	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	945.97	J/mol×K	979.45	Joback Method
cpg	966.23	J/mol×K	1019.07	Joback Method
cpg	987.09	J/mol×K	1058.68	Joback Method
cpg	1008.79	J/mol×K	1098.30	Joback Method
cpg	1031.63	J/mol×K	1137.92	Joback Method
cpg	1055.87	J/mol×K	1177.54	Joback Method
cpg	1081.79	J/mol×K	1217.15	Joback Method

Sources

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=R311029&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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