Maprotiline M(di-HO), diacetylated

Inchi: InChI=1S/C24H27NO4/c1-15(26)25(3)12-4-10-24-11-9-19(20-7-5-17(28)13-22(20)24)21-
InchiKey: DFNVBHIKRFICNK-UHFFFAOYSA-N
Formula: C24H27NO4
SMILES: CC(=O)Oc1ccc2c(c1)C1(CCCN(C)C(C)=O)CCC2c2ccc(O)cc21
Mol. weight [g/mol]: 393.48

Physical Properties

Property code	Value	Unit	Source
gf	80.66	kJ/mol	Joback Method
hf	-394.04	kJ/mol	Joback Method
hfus	52.19	kJ/mol	Joback Method
hvap	104.85	kJ/mol	Joback Method
log10ws	-5.01		Crippen Method
logp	4.101		Crippen Method
mcvol	304.640	ml/mol	McGowan Method
pc	1744.82	kPa	Joback Method
rinpol	2820.00		NIST Webbook
rinpol	2820.00		NIST Webbook
tb	1045.22	K	Joback Method
tc	1289.34	K	Joback Method
tf	783.74	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1058.24	J/mol×K	1045.22	Joback Method
cpg	1083.65	J/mol×K	1085.91	Joback Method
cpg	1110.77	J/mol×K	1126.59	Joback Method
cpg	1139.97	J/mol×K	1167.28	Joback Method
cpg	1171.62	J/mol×K	1207.97	Joback Method
cpg	1206.08	J/mol×K	1248.66	Joback Method
cpg	1243.71	J/mol×K	1289.34	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=R310977&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