Maprotiline M(tri-HO), triacetylated

Inchi: InChI=1S/C26H29NO6/c1-15(28)27(4)11-5-9-26-10-8-21(20-7-6-18(12-22(20)26)32-16(2
InchiKey: HLYOUXWTOSSKQS-UHFFFAOYSA-N
Formula: C26H29NO6
SMILES: CC(=O)Oc1ccc2c(c1)C1(CCCN(C)C(C)=O)CCC2c2c(O)cc(OC(C)=O)cc21
Mol. weight [g/mol]: 451.51

Physical Properties

Property code	Value	Unit	Source
gf	-146.05	kJ/mol	Joback Method
hf	-691.59	kJ/mol	Joback Method
hfus	59.77	kJ/mol	Joback Method
hvap	119.12	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.027		Crippen Method
mcvol	340.260	ml/mol	McGowan Method
pc	1531.86	kPa	Joback Method
rinpol	3200.00		NIST Webbook
rinpol	3200.00		NIST Webbook
tb	1172.25	K	Joback Method
tc	1435.18	K	Joback Method
tf	890.96	K	Joback Method
vc	1.242	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.36	J/mol×K	1172.25	Joback Method
cpg	1284.66	J/mol×K	1216.07	Joback Method
cpg	1320.73	J/mol×K	1259.89	Joback Method
cpg	1360.00	J/mol×K	1303.72	Joback Method
cpg	1402.90	J/mol×K	1347.54	Joback Method
cpg	1449.83	J/mol×K	1391.36	Joback Method
cpg	1501.24	J/mol×K	1435.18	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R311034&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

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