Maprotiline M(HO-anthryl), diacetylated

Inchi: InChI=1S/C24H27NO3/c1-17(26)25(3)16-8-13-23-14-15-24(28-18(2)27,21-11-6-4-9-19(2
InchiKey: PQYFNCMMKBDKQF-UHFFFAOYSA-N
Formula: C24H27NO3
SMILES: CC(=O)OC12CCC(CCCN(C)C(C)=O)(c3ccccc31)c1ccccc12
Mol. weight [g/mol]: 377.48

Physical Properties

Property code	Value	Unit	Source
gf	239.42	kJ/mol	Joback Method
hf	-190.02	kJ/mol	Joback Method
hfus	40.50	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-5.05		Crippen Method
logp	4.145		Crippen Method
mcvol	298.770	ml/mol	McGowan Method
pc	1621.98	kPa	Joback Method
rinpol	3096.00		NIST Webbook
rinpol	3096.00		NIST Webbook
tb	959.86	K	Joback Method
tc	1197.17	K	Joback Method
tf	683.40	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.00	J/mol×K	959.86	Joback Method
cpg	1019.14	J/mol×K	999.41	Joback Method
cpg	1045.87	J/mol×K	1038.96	Joback Method
cpg	1074.60	J/mol×K	1078.51	Joback Method
cpg	1105.74	J/mol×K	1118.07	Joback Method
cpg	1139.69	J/mol×K	1157.62	Joback Method
cpg	1176.85	J/mol×K	1197.17	Joback Method

Sources

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=R310982&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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