Clofedanol M (OH, -H2O), acetylated

Inchi: InChI=1S/C19H20ClNO2/c1-14(22)23-16-10-8-15(9-11-16)17(12-13-21(2)3)18-6-4-5-7-1
InchiKey: BMZFAEYMUILLJM-SFQUDFHCSA-N
Formula: C19H20ClNO2
SMILES: CC(=O)Oc1ccc(C(=CCN(C)C)c2ccccc2Cl)cc1
Mol. weight [g/mol]: 329.82

Physical Properties

Property code	Value	Unit	Source
gf	251.26	kJ/mol	Joback Method
hf	-70.95	kJ/mol	Joback Method
hfus	41.17	kJ/mol	Joback Method
hvap	79.39	kJ/mol	Joback Method
log10ws	-4.84		Crippen Method
logp	4.259		Crippen Method
mcvol	256.410	ml/mol	McGowan Method
pc	1816.95	kPa	Joback Method
rinpol	2370.00		NIST Webbook
rinpol	2370.00		NIST Webbook
tb	827.64	K	Joback Method
tc	1061.00	K	Joback Method
tf	497.28	K	Joback Method
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	721.43	J/mol×K	827.64	Joback Method
cpg	736.37	J/mol×K	866.53	Joback Method
cpg	750.16	J/mol×K	905.43	Joback Method
cpg	762.88	J/mol×K	944.32	Joback Method
cpg	774.61	J/mol×K	983.21	Joback Method
cpg	785.44	J/mol×K	1022.11	Joback Method
cpg	795.47	J/mol×K	1061.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120586&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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