Clofedanol N (nor, OH, -H2O), acetylated

Inchi: InChI=1S/C20H20ClNO3/c1-14(23)22(3)13-12-18(19-6-4-5-7-20(19)21)16-8-10-17(11-9-

InchiKey: KEKMPBIVPTVWBR-LDADJPATSA-N

Formula: C20H20ClNO3

SMILES: CC(=O)Oc1ccc(C(=CCN(C)C(C)=O)c2ccccc2Cl)cc1

Mol. weight [g/mol]: 357.83

Physical Properties

Property code	Value	Unit	Source
gf	130.76	kJ/mol	Joback Method
hf	-204.17	kJ/mol	Joback Method
hfus	45.36	kJ/mol	Joback Method
hvap	88.36	kJ/mol	Joback Method
log10ws	-5.03		Crippen Method
logp	4.175		Crippen Method
mcvol	272.070	ml/mol	McGowan Method
pc	1766.90	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	904.39	K	Joback Method
tc	1140.20	K	Joback Method
tf	558.48	K	Joback Method
vc	1.018	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.77	J/mol×K	904.39	Joback Method
cpg	802.97	J/mol×K	943.69	Joback Method
cpg	815.08	J/mol×K	982.99	Joback Method
cpg	826.19	J/mol×K	1022.30	Joback Method
cpg	836.38	J/mol×K	1061.60	Joback Method
cpg	845.77	J/mol×K	1100.90	Joback Method
cpg	854.42	J/mol×K	1140.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120591&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