Clofedanol M (nor, -H2O), acetylated

Inchi: InChI=1S/C18H18ClNO/c1-14(21)20(2)13-12-16(15-8-4-3-5-9-15)17-10-6-7-11-18(17)19
InchiKey: NVHQZWIRBQIPIF-FOWTUZBSSA-N
Formula: C18H18ClNO
SMILES: CC(=O)N(C)CC=C(c1ccccc1)c1ccccc1Cl
Mol. weight [g/mol]: 299.80

Physical Properties

Property code	Value	Unit	Source
gf	357.47	kJ/mol	Joback Method
hf	93.38	kJ/mol	Joback Method
hfus	37.78	kJ/mol	Joback Method
hvap	74.09	kJ/mol	Joback Method
log10ws	-4.72		Crippen Method
logp	4.250		Crippen Method
mcvol	236.450	ml/mol	McGowan Method
pc	2032.72	kPa	Joback Method
rinpol	2400.00		NIST Webbook
tb	777.36	K	Joback Method
tc	1016.82	K	Joback Method
tf	451.26	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.00	J/mol×K	777.36	Joback Method
cpg	655.39	J/mol×K	817.27	Joback Method
cpg	669.58	J/mol×K	857.18	Joback Method
cpg	682.69	J/mol×K	897.09	Joback Method
cpg	694.83	J/mol×K	937.00	Joback Method
cpg	706.14	J/mol×K	976.91	Joback Method
cpg	716.72	J/mol×K	1016.82	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120571&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