Clofedanol M (-H2O), acetylated

Inchi: InChI=1S/C17H18ClN/c1-19(2)13-12-15(14-8-4-3-5-9-14)16-10-6-7-11-17(16)18/h3-12H,
InchiKey: HCMDSXUJKIHBAB-NTCAYCPXSA-N
Formula: C17H18ClN
SMILES: CN(C)CC=C(c1ccccc1)c1ccccc1Cl
Mol. weight [g/mol]: 271.79

Physical Properties

Property code	Value	Unit	Source
gf	477.97	kJ/mol	Joback Method
hf	226.60	kJ/mol	Joback Method
hfus	33.59	kJ/mol	Joback Method
hvap	65.12	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	4.333		Crippen Method
mcvol	220.790	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	2085.00		NIST Webbook
rinpol	2085.00		NIST Webbook
tb	700.61	K	Joback Method
tc	939.56	K	Joback Method
tf	390.06	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.74	J/mol×K	700.61	Joback Method
cpg	586.94	J/mol×K	740.44	Joback Method
cpg	602.81	J/mol×K	780.26	Joback Method
cpg	617.47	J/mol×K	820.09	Joback Method
cpg	631.03	J/mol×K	859.91	Joback Method
cpg	643.61	J/mol×K	899.74	Joback Method
cpg	655.32	J/mol×K	939.56	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=R120566&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