Chlorprothixene M (nor-), monoacetylated

Inchi: InChI=1S/C19H18ClNOS/c1-13(22)21(2)11-5-7-15-16-6-3-4-8-18(16)23-19-10-9-14(20)1
InchiKey: SNMDHCOJSZRJJM-VIZOYTHASA-N
Formula: C19H18ClNOS
SMILES: CC(=O)N(C)CCC=C1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]: 343.87

Physical Properties

Property code	Value	Unit	Source
gf	440.84	kJ/mol	Joback Method
hf	162.96	kJ/mol	Joback Method
hfus	43.84	kJ/mol	Joback Method
hvap	84.25	kJ/mol	Joback Method
log10ws	-5.80		Crippen Method
logp	5.105		Crippen Method
mcvol	256.030	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	2945.00		NIST Webbook
rinpol	2945.00		NIST Webbook
tb	867.77	K	Joback Method
tc	1113.21	K	Joback Method
tf	626.12	K	Joback Method
vc	0.952	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.29	J/mol×K	867.77	Joback Method
cpg	724.03	J/mol×K	908.68	Joback Method
cpg	737.06	J/mol×K	949.58	Joback Method
cpg	749.52	J/mol×K	990.49	Joback Method
cpg	761.58	J/mol×K	1031.40	Joback Method
cpg	773.41	J/mol×K	1072.31	Joback Method
cpg	785.17	J/mol×K	1113.21	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=R310204&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