Chlorprothixene M (nor-dihydro-), monoacetylated

Inchi: InChI=1S/C19H20ClNOS/c1-13(22)21(2)11-5-7-15-16-6-3-4-8-18(16)23-19-10-9-14(20)1

InchiKey: UPEOGWOZHZRBRK-UHFFFAOYSA-N

Formula: C19H20ClNOS

SMILES: CC(=O)N(C)CCCC1c2ccccc2Sc2ccc(Cl)cc21

Mol. weight [g/mol]: 345.89

Physical Properties

Property code	Value	Unit	Source
gf	387.67	kJ/mol	Joback Method
hf	66.59	kJ/mol	Joback Method
hfus	44.59	kJ/mol	Joback Method
hvap	83.15	kJ/mol	Joback Method
log10ws	-5.74		Crippen Method
logp	5.195		Crippen Method
mcvol	260.330	ml/mol	McGowan Method
pc	1887.08	kPa	Joback Method
rinpol	2930.00		NIST Webbook
rinpol	2930.00		NIST Webbook
tb	856.46	K	Joback Method
tc	1096.61	K	Joback Method
tf	611.52	K	Joback Method
vc	0.968	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.11	J/mol×K	856.46	Joback Method
cpg	758.82	J/mol×K	896.48	Joback Method
cpg	772.62	J/mol×K	936.51	Joback Method
cpg	785.66	J/mol×K	976.53	Joback Method
cpg	798.06	J/mol×K	1016.56	Joback Method
cpg	809.97	J/mol×K	1056.58	Joback Method
cpg	821.53	J/mol×K	1096.61	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R310219&Units=SI

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