Chlorprothixene M (HO-dihydro-), monoacetylated

Inchi: InChI=1S/C20H22ClNO2S/c1-13(23)24-15-7-9-20-18(12-15)16(5-4-10-22(2)3)17-11-14(2
InchiKey: KIOLPMMETRQELR-UHFFFAOYSA-N
Formula: C20H22ClNO2S
SMILES: CC(=O)Oc1ccc2c(c1)C(CCCN(C)C)c1cc(Cl)ccc1S2
Mol. weight [g/mol]: 375.91

Physical Properties

Property code	Value	Unit	Source
gf	281.46	kJ/mol	Joback Method
hf	-97.74	kJ/mol	Joback Method
hfus	47.98	kJ/mol	Joback Method
hvap	88.45	kJ/mol	Joback Method
log10ws	-5.86		Crippen Method
logp	5.204		Crippen Method
mcvol	280.290	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2800.00		NIST Webbook
rinpol	2800.00		NIST Webbook
tb	906.74	K	Joback Method
tc	1142.51	K	Joback Method
tf	657.54	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	827.34	J/mol×K	906.74	Joback Method
cpg	841.74	J/mol×K	946.03	Joback Method
cpg	855.22	J/mol×K	985.33	Joback Method
cpg	867.89	J/mol×K	1024.62	Joback Method
cpg	879.85	J/mol×K	1063.92	Joback Method
cpg	891.21	J/mol×K	1103.21	Joback Method
cpg	902.08	J/mol×K	1142.51	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=R310195&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