Clopenthixol M (desalkyl-), monoacetylated

Inchi: InChI=1S/C18H16ClNOS/c1-12(21)20-10-4-6-14-15-5-2-3-7-17(15)22-18-9-8-13(19)11-1
InchiKey: IDQBOOJPVLAYIE-MKMNVTDBSA-N
Formula: C18H16ClNOS
SMILES: CC(=O)NCCC=C1c2ccccc2Sc2ccc(Cl)cc21
Mol. weight [g/mol]: 329.84

Physical Properties

Property code	Value	Unit	Source
gf	411.03	kJ/mol	Joback Method
hf	169.54	kJ/mol	Joback Method
hfus	43.33	kJ/mol	Joback Method
hvap	86.42	kJ/mol	Joback Method
log10ws	-6.00		Crippen Method
logp	4.763		Crippen Method
mcvol	241.940	ml/mol	McGowan Method
pc	2206.22	kPa	Joback Method
rinpol	3490.00		NIST Webbook
tb	882.62	K	Joback Method
tc	1133.11	K	Joback Method
tf	635.04	K	Joback Method
vc	0.912	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.35	J/mol×K	882.62	Joback Method
cpg	678.09	J/mol×K	924.37	Joback Method
cpg	690.18	J/mol×K	966.12	Joback Method
cpg	701.78	J/mol×K	1007.86	Joback Method
cpg	713.03	J/mol×K	1049.61	Joback Method
cpg	724.10	J/mol×K	1091.36	Joback Method
cpg	735.15	J/mol×K	1133.11	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=R310239&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