Clopenthixol M (desalkyl-dihydro-), monoacetylated

Inchi: InChI=1S/C18H18ClNOS/c1-12(21)20-10-4-6-14-15-5-2-3-7-17(15)22-18-9-8-13(19)11-1

InchiKey: LUCNRCZEQCNVKL-UHFFFAOYSA-N

Formula: C18H18ClNOS

SMILES: CC(=O)NCCCC1c2ccccc2Sc2ccc(Cl)cc21

Mol. weight [g/mol]: 331.86

Physical Properties

Property code	Value	Unit	Source
gf	357.86	kJ/mol	Joback Method
hf	73.17	kJ/mol	Joback Method
hfus	44.08	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-5.94		Crippen Method
logp	4.853		Crippen Method
mcvol	246.240	ml/mol	McGowan Method
pc	2083.12	kPa	Joback Method
rinpol	3450.00		NIST Webbook
rinpol	3450.00		NIST Webbook
tb	871.31	K	Joback Method
tc	1116.43	K	Joback Method
tf	620.44	K	Joback Method
vc	0.928	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.94	J/mol×K	871.31	Joback Method
cpg	713.60	J/mol×K	912.16	Joback Method
cpg	726.41	J/mol×K	953.02	Joback Method
cpg	738.50	J/mol×K	993.87	Joback Method
cpg	750.01	J/mol×K	1034.73	Joback Method
cpg	761.07	J/mol×K	1075.58	Joback Method
cpg	771.81	J/mol×K	1116.43	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=R310244&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

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