Tetrazepam M (hydroxy-), isomer 4, hydrolysis, acetylated

Inchi: InChI=1S/C18H20ClNO4/c1-11(21)20(3)17-9-6-14(19)10-16(17)18(23)13-4-7-15(8-5-13)

InchiKey: YOTCKTVZLVRITG-UHFFFAOYSA-N

Formula: C18H20ClNO4

SMILES: CC(=O)OC1CC=C(C(=O)c2cc(Cl)ccc2N(C)C(C)=O)CC1

Mol. weight [g/mol]: 349.81

Physical Properties

Property code	Value	Unit	Source
gf	-154.30	kJ/mol	Joback Method
hf	-518.80	kJ/mol	Joback Method
hfus	41.51	kJ/mol	Joback Method
hvap	89.72	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.547		Crippen Method
mcvol	258.360	ml/mol	McGowan Method
pc	1913.58	kPa	Joback Method
rinpol	2560.00		NIST Webbook
tb	905.47	K	Joback Method
tc	1139.86	K	Joback Method
tf	599.15	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.20	J/mol×K	905.47	Joback Method
cpg	790.04	J/mol×K	944.54	Joback Method
cpg	801.52	J/mol×K	983.60	Joback Method
cpg	811.70	J/mol×K	1022.67	Joback Method
cpg	820.60	J/mol×K	1061.73	Joback Method
cpg	828.29	J/mol×K	1100.80	Joback Method
cpg	834.81	J/mol×K	1139.86	Joback Method

Sources

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=R313545&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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