Tetrazepam M (norhydroxy-), hydrolysis, acetylated

Inchi: InChI=1S/C17H18ClNO4/c1-10(20)19-15-8-7-12(18)9-14(15)17(22)13-5-3-4-6-16(13)23-

InchiKey: FKYVTMBWEWJAOV-UHFFFAOYSA-N

Formula: C17H18ClNO4

SMILES: CC(=O)Nc1ccc(Cl)cc1C(=O)C1=CCCCC1OC(C)=O

Mol. weight [g/mol]: 335.78

Physical Properties

Property code	Value	Unit	Source
gf	-184.11	kJ/mol	Joback Method
hf	-512.22	kJ/mol	Joback Method
hfus	41.00	kJ/mol	Joback Method
hvap	91.89	kJ/mol	Joback Method
log10ws	-4.67		Crippen Method
logp	3.523		Crippen Method
mcvol	244.270	ml/mol	McGowan Method
pc	2113.89	kPa	Joback Method
rinpol	2500.00		NIST Webbook
tb	920.32	K	Joback Method
tc	1159.22	K	Joback Method
tf	608.07	K	Joback Method
vc	0.918	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.32	J/mol×K	920.32	Joback Method
cpg	742.95	J/mol×K	960.14	Joback Method
cpg	753.21	J/mol×K	999.95	Joback Method
cpg	762.13	J/mol×K	1039.77	Joback Method
cpg	769.75	J/mol×K	1079.59	Joback Method
cpg	776.11	J/mol×K	1119.40	Joback Method
cpg	781.23	J/mol×K	1159.22	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R313550&Units=SI
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

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