Clonazepam M (amino-), hydrolysis, acetylated

Inchi: InChI=1S/C17H15ClN2O3/c1-10(21)19-12-7-8-16(20-11(2)22)14(9-12)17(23)13-5-3-4-6-
InchiKey: BOCLGTUHWYBPNT-UHFFFAOYSA-N
Formula: C17H15ClN2O3
SMILES: CC(=O)Nc1ccc(NC(C)=O)c(C(=O)c2ccccc2Cl)c1
Mol. weight [g/mol]: 330.77

Physical Properties

Property code	Value	Unit	Source
gf	68.28	kJ/mol	Joback Method
hf	-202.10	kJ/mol	Joback Method
hfus	45.89	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-4.52		Crippen Method
logp	3.488		Crippen Method
mcvol	239.780	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		NIST Webbook
tb	956.04	K	Joback Method
tc	1200.04	K	Joback Method
tf	656.78	K	Joback Method
vc	0.908	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	688.97	J/mol×K	956.04	Joback Method
cpg	698.58	J/mol×K	996.71	Joback Method
cpg	707.14	J/mol×K	1037.37	Joback Method
cpg	714.73	J/mol×K	1078.04	Joback Method
cpg	721.42	J/mol×K	1118.71	Joback Method
cpg	727.28	J/mol×K	1159.38	Joback Method
cpg	732.36	J/mol×K	1200.04	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=R312899&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