Nitrazepam M (amino-), hydrolysis, acetylated

Inchi: InChI=1S/C17H16N2O3/c1-11(20)18-14-8-9-16(19-12(2)21)15(10-14)17(22)13-6-4-3-5-7
InchiKey: OTPSWBRNSBDCMB-UHFFFAOYSA-N
Formula: C17H16N2O3
SMILES: CC(=O)Nc1ccc(NC(C)=O)c(C(=O)c2ccccc2)c1
Mol. weight [g/mol]: 296.32

Physical Properties

Property code	Value	Unit	Source
gf	89.84	kJ/mol	Joback Method
hf	-174.89	kJ/mol	Joback Method
hfus	42.09	kJ/mol	Joback Method
hvap	92.42	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	2.834		Crippen Method
mcvol	227.540	ml/mol	McGowan Method
pc	2492.52	kPa	Joback Method
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
rinpol	2985.00		NIST Webbook
tb	913.63	K	Joback Method
tc	1154.03	K	Joback Method
tf	614.34	K	Joback Method
vc	0.860	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.93	J/mol×K	913.63	Joback Method
cpg	682.83	J/mol×K	953.70	Joback Method
cpg	692.65	J/mol×K	993.76	Joback Method
cpg	701.45	J/mol×K	1033.83	Joback Method
cpg	709.31	J/mol×K	1073.90	Joback Method
cpg	716.31	J/mol×K	1113.97	Joback Method
cpg	722.50	J/mol×K	1154.03	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=R313327&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