Diazepam, M(HO-), acid hydrolyzed, acetylated

Inchi: InChI=1S/C18H16ClNO4/c1-11(21)20(3)16-9-8-13(19)10-15(16)18(23)14-6-4-5-7-17(14)

InchiKey: TYJLUIQZXUESTG-UHFFFAOYSA-N

Formula: C18H16ClNO4

SMILES: CC(=O)Oc1ccccc1C(=O)c1cc(Cl)ccc1N(C)C(C)=O

Mol. weight [g/mol]: 345.78

Physical Properties

Property code	Value	Unit	Source
gf	-96.30	kJ/mol	Joback Method
hf	-394.37	kJ/mol	Joback Method
hfus	42.49	kJ/mol	Joback Method
hvap	91.28	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.479		Crippen Method
mcvol	249.760	ml/mol	McGowan Method
pc	2073.65	kPa	Joback Method
rinpol	2600.00		NIST Webbook
rinpol	2600.00		NIST Webbook
tb	913.44	K	Joback Method
tc	1151.35	K	Joback Method
tf	617.43	K	Joback Method
vc	0.930	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	711.26	J/mol×K	913.44	Joback Method
cpg	722.20	J/mol×K	953.09	Joback Method
cpg	731.98	J/mol×K	992.74	Joback Method
cpg	740.65	J/mol×K	1032.39	Joback Method
cpg	748.25	J/mol×K	1072.04	Joback Method
cpg	754.85	J/mol×K	1111.70	Joback Method
cpg	760.50	J/mol×K	1151.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R255573&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

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