

Clobazam M (norhydroxymethoxy-), hydrolysis, acetylated

Inchi:	InChI=1S/C19H19ClN2O5/c1-11(23)21-16-7-5-14(20)9-18(16)22(12(2)24)17-8-6-15(27-1
InchiKey:	GHTJWULURLONXS-UHFFFAOYSA-N
Formula:	C19H19ClN2O5
SMILES:	COc1cc(OC(C)=O)ccc1N(C(C)=O)c1cc(Cl)ccc1NC(C)=O
Mol. weight [g/mol]:	390.82

Physical Properties

Property code	Value	Unit	Source
gf	-113.12	kJ/mol	Joback Method
hf	-505.23	kJ/mol	Joback Method
hfus	50.98	kJ/mol	Joback Method
hvap	103.01	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	3.917		Crippen Method
mcvol	279.700	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinsol	2615.00		NIST Webbook
tb	1013.89	K	Joback Method
tc	1252.79	K	Joback Method
tf	716.11	K	Joback Method
vc	1.040	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.03	J/molxK	1013.89	Joback Method
cpg	849.95	J/molxK	1053.71	Joback Method
cpg	857.49	J/molxK	1093.52	Joback Method
cpg	863.69	J/molxK	1133.34	Joback Method
cpg	868.57	J/molxK	1173.16	Joback Method
cpg	872.18	J/molxK	1212.97	Joback Method
cpg	874.55	J/molxK	1252.79	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R312879&Units=SI

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
mccvol:	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

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