

Clobazam, hydrolysis

Other names:	Clobazam, hydrolysis
Inchi:	InChI=1S/C13H13ClN2/c1-15-12-8-7-10(14)9-13(12)16-11-5-3-2-4-6-11/h2-9,15-16H,1H
InchiKey:	YFSSUNICRFFYOV-UHFFFAOYSA-N
Formula:	C13H13ClN2
SMILES:	CNc1ccc(Cl)cc1Nc1ccccc1
Mol. weight [g/mol]:	232.71

Physical Properties

Property code	Value	Unit	Source
af	0.5843		Cheméo Relay (1.0)
gf	430.99	kJ/mol	Joback Method
hf	157.45	kJ/mol	Cheméo Relay (1.0)
hfus	31.13	kJ/mol	Joback Method
hvap	93.54	kJ/mol	Cheméo Relay (1.0)
ie	6.99	eV	Cheméo Relay (1.0)
log10ws	-4.11		Cheméo Relay (1.0)
logp	4.125		Crippen Method
mcvol	178.710	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
rinpol	2225.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2225.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	626.21	K	Cheméo Relay (1.0)
tc	948.42	K	Cheméo Relay (1.0)
tf	381.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.00	J/mol×K	697.93	Joback Method
cpg	463.01	J/mol×K	738.68	Joback Method
cpg	475.89	J/mol×K	779.43	Joback Method
cpg	487.71	J/mol×K	820.17	Joback Method

cpg	498.53	J/mol×K	860.92	Joback Method
cpg	508.42	J/mol×K	901.67	Joback Method
cpg	517.47	J/mol×K	942.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R17896&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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