

Clorazepate

Other names:	Clorazepic acid Chlorazepate
Inchi:	InChI=1S/C16H11ClN2O3/c17-10-6-7-12-11(8-10)13(9-4-2-1-3-5-9)19-14(16(21)22)15(2
InchiKey:	XDDJGVMJFWAHJX-UHFFFAOYSA-N
Formula:	C16H11ClN2O3
SMILES:	O=C(O)C1N=C(c2ccccc2)c2cc(Cl)ccc2NC1=O
Mol. weight [g/mol]:	314.72

Physical Properties

Property code	Value	Unit	Source
gf	150.51	kJ/mol	Joback Method
hf	-126.13	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	103.32	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	2.583		Crippen Method
mcvol	214.830	ml/mol	McGowan Method
pc	3295.37	kPa	Joback Method
rinpol	2655.00		NIST Webbook
rinpol	2701.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2655.00		NIST Webbook
rinpol	2701.00		NIST Webbook
tb	1001.77	K	Joback Method
tc	1266.49	K	Joback Method
tf	757.60	K	Joback Method
vc	0.809	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	651.88	J/molxK	1001.77	Joback Method
cpg	659.03	J/molxK	1045.89	Joback Method

cpg	664.36	J/mol×K	1090.01	Joback Method
cpg	667.86	J/mol×K	1134.13	Joback Method
cpg	669.54	J/mol×K	1178.25	Joback Method
cpg	669.40	J/mol×K	1222.37	Joback Method
cpg	667.44	J/mol×K	1266.49	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R17056&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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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