

Nortetrazepam

Other names:	7-Chloro-5-(1-cyclohexen-1-yl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one CB-4260
Inchi:	InChI=1S/C15H15ClN2O/c16-11-6-7-13-12(8-11)15(17-9-14(19)18-13)10-4-2-1-3-5-10/h
InchiKey:	FDRMSENAXZDFTN-UHFFFAOYSA-N
Formula:	C15H15ClN2O
SMILES:	O=C1CN=C(C2=CCCCC2)c2cc(Cl)ccc2N1
Mol. weight [g/mol]:	274.75
CAS:	10379-11-0

Physical Properties

Property code	Value	Unit	Source
gf	355.62	kJ/mol	Joback Method
hf	64.10	kJ/mol	Joback Method
hfus	31.60	kJ/mol	Joback Method
hvap	77.40	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.582		Crippen Method
mvol	201.900	ml/mol	McGowan Method
pc	2953.69	kPa	Joback Method
rinpol	2520.00		NIST Webbook
rinpol	2520.00		NIST Webbook
tb	839.19	K	Joback Method
tc	1126.29	K	Joback Method
tf	638.30	K	Joback Method
vc	0.757	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	601.86	J/mol×K	839.19	Joback Method
cpg	618.17	J/mol×K	887.04	Joback Method
cpg	632.34	J/mol×K	934.89	Joback Method
cpg	644.39	J/mol×K	982.74	Joback Method
cpg	654.33	J/mol×K	1030.59	Joback Method

cpg	662.15	J/mol×K	1078.44	Joback Method
cpg	667.87	J/mol×K	1126.29	Joback Method

Sources

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=C10379110&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpolar:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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