Delorazepam

Other names:	2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(2-chlorophenyl)-1,3-dihydro- B1, Benzodiazepine Chlordemethyldiazepam Cl-DMDZ Ro 5-3027 2H-1,4-Benzodiazepin-2-one, 1,3-dihydro-7-chloro-5-(2-chlorophenyl)- 2H-1,4-Benzodiazepin-2-one, 7-chloro-5-(o-chlorophenyl)-1,3-dihydro- 7-Chloro-5-(2-chlorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one Chlordesmethyldiazepam Clordesmetildiazepam 1,3-Dihydro-7-chloro-5-(o-chlorophenyl)-2H-1,4-benzodiazepin-2-one EN RV-12165 7-Chloro-5-(o-chlorophenyl)-1,3-dihydro-2H-1,4-benzodiazepin-2-one 2'-Chloronordiazepam NSC 169895 EN [Anticonvulsant]
Inchi:	InChI=1S/C15H10Cl2N2O/c16-9-5-6-13-11(7-9)15(18-8-14(20)19-13)10-3-1-2-4-12(10)1
InchiKey:	CHIFCDOIPRCHCF-UHFFFAOYSA-N
Formula:	C15H10Cl2N2O
SMILES:	O=C1CN=C(c2ccccc2Cl)c2cc(Cl)ccc2N1
Mol. weight [g/mol]:	305.16
CAS:	2894-67-9

Physical Properties

Property code	Value	Unit	Source
gf	393.98	kJ/mol	Joback Method
hf	152.45	kJ/mol	Joback Method
hfus	37.85	kJ/mol	Joback Method
hvap	83.03	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.783		Crippen Method
mcvol	205.540	ml/mol	McGowan Method
pc	3018.96	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
rinpol	2571.00		NIST Webbook

rinpol	2571.00		NIST Webbook
rinpol	2593.00		NIST Webbook
rinpol	2569.00		NIST Webbook
tb	879.92	K	Joback Method
tc	1173.17	K	Joback Method
tf	682.26	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.40	J/mol×K	879.92	Joback Method
cpg	576.60	J/mol×K	928.80	Joback Method
cpg	586.83	J/mol×K	977.67	Joback Method
cpg	595.09	J/mol×K	1026.55	Joback Method
cpg	601.38	J/mol×K	1075.42	Joback Method
cpg	605.70	J/mol×K	1124.30	Joback Method
cpg	608.06	J/mol×K	1173.17	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=C2894679&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume