

Diazoxide

Other names:	2H-1,2,4-Benzothiadiazine, 7-chloro-3-methyl-, 1,1-dioxide
	4H-1,2,4-Benzothiadiazine, 7-chloro-3-methyl-, 1,1-dioxide
	7-Chloro-3-methyl-2H-1,2,4-benzothiadiazine 1,1-dioxide
	7-Chloro-3-methyl-2H-1,2,4-benzothiadiazine 1,1-dioxide (diazoxide)
	7-Cloro-3-metil-2H-1,2,4-benzotiodiazina-1,1-diossido
	Diazossido
	Dizoxide
	Eudemine
	Eudemine injection
	Hyperstat
	Hypertonalum
	Mutabase
	NSC 76130
	NSC-64198
	Proglycem
	Proglycem
Inchi:	InChI=1S/C8H7ClN2O2S/c1-5-10-7-3-2-6(9)4-8(7)14(12,13)11-5/h2-4H,1H3,(H,10,11)
InchiKey:	GDLBFKVLRPITMI-UHFFFAOYSA-N
Formula:	C8H7ClN2O2S
SMILES:	CC1=NS(=O)(=O)c2cc(Cl)ccc2N1
Mol. weight [g/mol]:	230.67
CAS:	364-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-82.92	kJ/mol	Joback Method
hf	-218.49	kJ/mol	Joback Method
hfus	35.37	kJ/mol	Joback Method
hvap	73.33	kJ/mol	Joback Method
log10ws	-3.36		Aqueous Solubility Prediction Method
logp	1.873		Crippen Method
mcpvol	144.950	ml/mol	McGowan Method
pc	5446.55	kPa	Joback Method
tb	605.41	K	Joback Method

tc	850.58	K	Joback Method
tf	557.42	K	Joback Method
vc	0.565	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.73	J/mol×K	605.41	Joback Method
cpg	341.30	J/mol×K	646.27	Joback Method
cpg	352.91	J/mol×K	687.13	Joback Method
cpg	363.57	J/mol×K	727.99	Joback Method
cpg	373.29	J/mol×K	768.85	Joback Method
cpg	382.08	J/mol×K	809.71	Joback Method
cpg	389.95	J/mol×K	850.58	Joback Method
hfust	34.10	kJ/mol	600.40	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C364987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx

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
hfust:	Enthalpy of fusion at a given temperature
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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