Chlornidine

Other names: Benzenamine, N,N-bis(2-chloroethyl)-4-methyl-2,6-dinitro-
p-Toluidine, N,N-bis(2-chloroethyl)-2,6-dinitro-
AN 5647
AN 56477
Torpedo

Inchi: InChI=1S/C11H13Cl2N3O4/c1-8-6-9(15(17)18)11(10(7-8)16(19)20)14(4-2-12)5-3-13/h6-

InchiKey: XKUWFOYPQIVFMM-UHFFFAOYSA-N

Formula: C11H13Cl2N3O4

SMILES: Cc1cc([N+](=O)[O-])c(N(CCCl)CCCl)c([N+](=O)[O-])c1

Mol. weight [g/mol]: 322.14

CAS: 26389-78-6

Physical Properties

Property code	Value	Unit	Source
gf	283.28	kJ/mol	Joback Method
hf	-53.72	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	88.34	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	3.095		Crippen Method
mcvol	211.390	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
tb	883.68	K	Joback Method
tc	1134.07	K	Joback Method
tf	657.24	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.39	J/mol×K	883.68	Joback Method
cpg	590.43	J/mol×K	925.41	Joback Method
cpg	599.59	J/mol×K	967.14	Joback Method
cpg	607.92	J/mol×K	1008.88	Joback Method

cpg	615.51	J/mol×K	1050.61	Joback Method
cpg	622.43	J/mol×K	1092.34	Joback Method
cpg	628.75	J/mol×K	1134.07	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=C26389786&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume