

Diloxanide

Other names:	Acetamide, 2,2-dichloro-N-(4-hydroxyphenyl)-N-methyl- Acetanilide, 2,2-dichloro-4'-hydroxy-N-methyl- Amebamida Ame-boots Diloxanid Entamide M & B 4453 RD 3803 2,2-Dichloro-4'-hydroxy-N-methylacetanilide 2,2-Dichloro-N-(4-hydroxyphenyl)-N-methylacetamide
Inchi:	InChI=1S/C9H9Cl2NO2/c1-12(9(14)8(10)11)6-2-4-7(13)5-3-6/h2-5,8,13H,1H3
InchiKey:	GZZZSOOGQLOEOB-UHFFFAOYSA-N
Formula:	C9H9Cl2NO2
SMILES:	CN(C(=O)C(Cl)Cl)c1ccc(O)cc1
Mol. weight [g/mol]:	234.08
CAS:	579-38-4

Physical Properties

Property code	Value	Unit	Source
gf	-61.75	kJ/mol	Joback Method
hf	-251.68	kJ/mol	Joback Method
hfus	28.38	kJ/mol	Joback Method
hvap	68.09	kJ/mol	Joback Method
log10ws	-2.03		Crippen Method
logp	2.159		Crippen Method
mcvol	155.810	ml/mol	McGowan Method
pc	3872.29	kPa	Joback Method
tb	653.35	K	Joback Method
tc	892.19	K	Joback Method
tf	456.57	K	Joback Method
vc	0.513	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	361.93	J/mol×K	653.35	Joback Method
cpg	372.22	J/mol×K	693.16	Joback Method
cpg	381.66	J/mol×K	732.96	Joback Method
cpg	390.37	J/mol×K	772.77	Joback Method
cpg	398.46	J/mol×K	812.58	Joback Method
cpg	406.05	J/mol×K	852.38	Joback Method
cpg	413.24	J/mol×K	892.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C579384&Units=SI
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

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

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