

Clorgiline

Other names:	2-Propynylamine, N-(3-(2,4-dichlorophenoxy)propyl)-N-methyl- Chlorgiline Clorgyline N-(3-(2,4-Dichlorophenoxy)propyl)-N-methyl-2-propynylamine M & B 9302 2-Propyn-1-amine, N-(3-(2,4-dichlorophenoxy)propyl)-N-methyl-
Inchi:	InChI=1S/C13H15Cl2NO/c1-3-7-16(2)8-4-9-17-13-6-5-11(14)10-12(13)15/h1,5-6,10H,4,7
InchiKey:	BTFHLQRNAMS NLC-UHFFFAOYSA-N
Formula:	C13H15Cl2NO
SMILES:	C#CCN(C)CCCOc1ccc(Cl)cc1Cl
Mol. weight [g/mol]:	272.17
CAS:	17780-72-2

Physical Properties

Property code	Value	Unit	Source
gf	356.72	kJ/mol	Joback Method
hf	97.67	kJ/mol	Joback Method
hfus	38.27	kJ/mol	Joback Method
hvap	61.21	kJ/mol	Joback Method
log10ws	-3.84		Crippen Method
logp	3.327		Crippen Method
mcvol	202.000	ml/mol	McGowan Method
pc	2246.13	kPa	Joback Method
rinpol	1883.00		NIST Webbook
tb	633.32	K	Joback Method
tc	848.84	K	Joback Method
tf	449.24	K	Joback Method
vc	0.751	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.84	J/mol×K	633.32	Joback Method
cpg	487.89	J/mol×K	669.24	Joback Method

cpg	501.06	J/mol×K	705.16	Joback Method
cpg	513.38	J/mol×K	741.08	Joback Method
cpg	524.91	J/mol×K	777.00	Joback Method
cpg	535.66	J/mol×K	812.92	Joback Method
cpg	545.69	J/mol×K	848.84	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17780722&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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