N,N-Bis(4-chlorobenzyl)hydroxylamine

Inchi: InChI=1S/C14H13Cl2NO/c15-13-5-1-11(2-6-13)9-17(18)10-12-3-7-14(16)8-4-12/h1-8,18
InchiKey: LJISSWQMTWDSGS-UHFFFAOYSA-N
Formula: C14H13Cl2NO
SMILES: ON(Cc1ccc(Cl)cc1)Cc1ccc(Cl)cc1
Mol. weight [g/mol]: 282.17
CAS: 40861-08-3

Physical Properties

Property code	Value	Unit	Source
gf	222.66	kJ/mol	Joback Method
hf	1.65	kJ/mol	Joback Method
hfus	34.82	kJ/mol	Joback Method
hvap	80.13	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.385		Crippen Method
mcvol	200.930	ml/mol	McGowan Method
pc	2729.71	kPa	Joback Method
tb	762.52	K	Joback Method
tc	986.76	K	Joback Method
tf	478.55	K	Joback Method
vc	0.739	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	512.25	J/mol×K	762.52	Joback Method
cpg	523.71	J/mol×K	799.89	Joback Method
cpg	534.29	J/mol×K	837.27	Joback Method
cpg	544.05	J/mol×K	874.64	Joback Method
cpg	553.06	J/mol×K	912.02	Joback Method
cpg	561.39	J/mol×K	949.39	Joback Method
cpg	569.11	J/mol×K	986.76	Joback Method

Sources

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=C40861083&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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