

Benzenemethanol, 2-chloro-«alpha»-[[[(1-methylethyl)amino]methyl]-

Other names:

Clorprenaline
Isoprophenamineisoprofenamine
o-Chloro-«alpha»-[(isopropylamino)methyl]benzyl alcohol
Chlorprenaline

Inchi: InChI=1S/C11H16ClNO/c1-8(2)13-7-11(14)9-5-3-4-6-10(9)12/h3-6,8,11,13-14H,7H2,1-2H

InchiKey: SSMSBSWKLKXGG-UHFFFAOYSA-N

Formula: C11H16ClNO

SMILES: CC(C)NCC(O)c1ccccc1Cl

Mol. weight [g/mol]: 213.70

CAS: 3811-25-4

Physical Properties

Property code	Value	Unit	Source
gf	80.28	kJ/mol	Joback Method
hf	-170.37	kJ/mol	Joback Method
hfus	24.24	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	2.371		Crippen Method
mcvol	170.180	ml/mol	McGowan Method
pc	2847.48	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1556.00		NIST Webbook
rinpol	1604.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	661.64	K	Joback Method
tc	864.63	K	Joback Method
tf	366.07	K	Joback Method
vc	0.634	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.37	J/mol×K	661.64	Joback Method
cpg	447.88	J/mol×K	695.47	Joback Method
cpg	459.62	J/mol×K	729.30	Joback Method
cpg	470.64	J/mol×K	763.13	Joback Method
cpg	480.95	J/mol×K	796.96	Joback Method
cpg	490.61	J/mol×K	830.80	Joback Method
cpg	499.64	J/mol×K	864.63	Joback Method

Sources

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=C3811254&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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