

Benzeneethanamine, 2-chloro-

Other names:	o-Chlorophenethylamine 2-(O-Chlorophenyl)ethylamine 2-(2-Chlorophenyl)ethylamine 2-Chlorophenethylamine
Inchi:	InChI=1S/C8H10ClN/c9-8-4-2-1-3-7(8)5-6-10/h1-4H,5-6,10H2
InchiKey:	RZBOMSOHMOVUES-UHFFFAOYSA-N
Formula:	C8H10ClN
SMILES:	NCCc1ccccc1Cl
Mol. weight [g/mol]:	155.62
CAS:	13078-80-3

Physical Properties

Property code	Value	Unit	Source
gf	173.78	kJ/mol	Joback Method
hf	34.66	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	51.37	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	1.841		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3673.09	kPa	Joback Method
tb	524.06	K	Joback Method
tc	753.66	K	Joback Method
tf	332.04	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.53	J/mol×K	524.06	Joback Method
cpg	265.37	J/mol×K	562.33	Joback Method
cpg	276.44	J/mol×K	600.59	Joback Method
cpg	286.78	J/mol×K	638.86	Joback Method
cpg	296.41	J/mol×K	677.13	Joback Method

cpg	305.38	J/mol×K	715.39	Joback Method
cpg	313.73	J/mol×K	753.66	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	393.20	K	2.00	NIST Webbook

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=C13078803&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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