

2-Chloro-6-methylbenzylamine

Inchi:	InChI=1S/C8H10ClN/c1-6-3-2-4-8(9)7(6)5-10/h2-4H,5,10H2,1H3
InchiKey:	WPQIAYXZZULKMV-UHFFFAOYSA-N
Formula:	C8H10ClN
SMILES:	Cc1cccc(Cl)c1CN
Mol. weight [g/mol]:	155.62
CAS:	57264-46-7

Physical Properties

Property code	Value	Unit	Source
gf	164.15	kJ/mol	Joback Method
hf	23.19	kJ/mol	Joback Method
hfus	19.13	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-2.95		Crippen Method
logp	2.107		Crippen Method
mcvol	122.040	ml/mol	McGowan Method
pc	3607.21	kPa	Joback Method
tb	529.04	K	Joback Method
tc	759.83	K	Joback Method
tf	344.56	K	Joback Method
vc	0.454	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	253.03	J/mol×K	529.04	Joback Method
cpg	264.50	J/mol×K	567.51	Joback Method
cpg	275.27	J/mol×K	605.97	Joback Method
cpg	285.37	J/mol×K	644.44	Joback Method
cpg	294.82	J/mol×K	682.90	Joback Method
cpg	303.66	J/mol×K	721.37	Joback Method
cpg	311.90	J/mol×K	759.83	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57264467&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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