

Benzaldehyde, 2-chloro-4-dimethylamino-

Other names:	2-chloro-4-dimethylaminobenzaldehyde
Inchi:	InChI=1S/C9H10ClNO/c1-11(2)8-4-3-7(6-12)9(10)5-8/h3-6H,1-2H3
InchiKey:	XSQFAWMDRFSIMY-UHFFFAOYSA-N
Formula:	C9H10ClNO
SMILES:	CN(C)c1ccc(C=O)c(Cl)c1
Mol. weight [g/mol]:	183.63
CAS:	1424-66-4

Physical Properties

Property code	Value	Unit	Source
gf	117.38	kJ/mol	Joback Method
hf	-49.29	kJ/mol	Joback Method
hfus	21.84	kJ/mol	Joback Method
hvap	52.38	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.219		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	540.49	K	Joback Method
tc	757.58	K	Joback Method
tf	347.04	K	Joback Method
vc	0.515	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	292.56	J/mol×K	540.49	Joback Method
cpg	304.45	J/mol×K	576.67	Joback Method
cpg	315.58	J/mol×K	612.85	Joback Method
cpg	325.98	J/mol×K	649.03	Joback Method
cpg	335.70	J/mol×K	685.22	Joback Method
cpg	344.76	J/mol×K	721.40	Joback Method
cpg	353.20	J/mol×K	757.58	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1424664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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