Carbamic acid, N-methyl-, 2,3-dichlorobenzyl ester

Other names: 2,3-Dichlorobenzyl, N-methylcarbamate
Benzenemethanol, 2,3-dichloro-, methylcarbamate
2,3-Dichlorobenzyl methylcarbamate
2,3-Sirmate

Inchi: InChI=1S/C9H9Cl2NO2/c1-12-9(13)14-5-6-3-2-4-7(10)8(6)11/h2-4H,5H2,1H3,(H,12,13)

InchiKey: SESJCOBCXSACPH-UHFFFAOYSA-N

Formula: C9H9Cl2NO2

SMILES: CNC(=O)OCc1cccc(Cl)c1Cl

Mol. weight [g/mol]: 234.08

CAS: 2328-31-6

Physical Properties

Property code	Value	Unit	Source
gf	-50.34	kJ/mol	Joback Method
hf	-238.31	kJ/mol	Joback Method
hfus	28.61	kJ/mol	Joback Method
hvap	63.59	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	2.849		Crippen Method
mcvol	155.810	ml/mol	McGowan Method
pc	3100.18	kPa	Joback Method
tb	643.28	K	Joback Method
tc	869.01	K	Joback Method
tf	427.31	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.24	J/mol×K	643.28	Joback Method
cpg	357.77	J/mol×K	680.90	Joback Method
cpg	367.60	J/mol×K	718.52	Joback Method
cpg	376.74	J/mol×K	756.15	Joback Method
cpg	385.20	J/mol×K	793.77	Joback Method

cpg	392.99	J/mol×K	831.39	Joback Method
cpg	400.12	J/mol×K	869.01	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=C2328316&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume