

Benzyl alcohol, m-chloro-alpha-dichloromethyl-

Inchi:	InChI=1S/C8H7Cl3O/c9-6-3-1-2-5(4-6)7(12)8(10)11/h1-4,7-8,12H
InchiKey:	INLMRTPMNPOFAV-UHFFFAOYSA-N
Formula:	C8H7Cl3O
SMILES:	OC(c1cccc(Cl)c1)C(Cl)Cl
Mol. weight [g/mol]:	225.50
CAS:	27683-61-0

Physical Properties

Property code	Value	Unit	Source
gf	-58.23	kJ/mol	Joback Method
hf	-193.40	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	65.40	kJ/mol	Joback Method
log10ws	-3.59		Crippen Method
logp	3.177		Crippen Method
mcvol	142.410	ml/mol	McGowan Method
pc	3572.80	kPa	Joback Method
tb	617.69	K	Joback Method
tc	838.24	K	Joback Method
tf	339.44	K	Joback Method
vc	0.529	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.50	J/molxK	617.69	Joback Method
cpg	300.15	J/molxK	654.45	Joback Method
cpg	308.16	J/molxK	691.21	Joback Method
cpg	315.56	J/molxK	727.97	Joback Method
cpg	322.40	J/molxK	764.73	Joback Method
cpg	328.70	J/molxK	801.48	Joback Method
cpg	334.51	J/molxK	838.24	Joback Method
dvisc	0.0066807	Paxs	339.44	Joback Method
dvisc	0.0020363	Paxs	385.81	Joback Method

dvisc	0.0008009	Paxs	432.19	Joback Method
dvisc	0.0003775	Paxs	478.57	Joback Method
dvisc	0.0002032	Paxs	524.94	Joback Method
dvisc	0.0001210	Paxs	571.32	Joback Method
dvisc	0.0000778	Paxs	617.69	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=C27683610&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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