

Benzene, 1-(1-chloroethyl)-4-(chloromethyl)-

Other names:	4-(1-Chloroethyl)benzyl chloride p-(Alpha-chloroethyl)benzyl chloride Benzene, 1-chloromethyl-4-(1-chloroethyl)-
Inchi:	InChI=1S/C9H10Cl2/c1-7(11)9-4-2-8(6-10)3-5-9/h2-5,7H,6H2,1H3
InchiKey:	OPVAKHQEJWPSQB-UHFFFAOYSA-N
Formula:	C9H10Cl2
SMILES:	CC(Cl)c1ccc(CCl)cc1
Mol. weight [g/mol]:	189.08
CAS:	54789-30-9

Physical Properties

Property code	Value	Unit	Source
gf	101.38	kJ/mol	Joback Method
hf	-40.79	kJ/mol	Joback Method
hfus	17.59	kJ/mol	Joback Method
hvap	46.95	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.725		Crippen Method
mcvol	138.390	ml/mol	McGowan Method
pc	2979.54	kPa	Joback Method
tb	511.40	K	Joback Method
tc	737.08	K	Joback Method
tf	274.97	K	Joback Method
vc	0.523	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.89	J/molxK	511.40	Joback Method
cpg	281.43	J/molxK	549.01	Joback Method
cpg	293.17	J/molxK	586.63	Joback Method
cpg	304.13	J/molxK	624.24	Joback Method
cpg	314.35	J/molxK	661.86	Joback Method
cpg	323.88	J/molxK	699.47	Joback Method

cpg	332.74	J/mol×K	737.08	Joback Method
dvisc	0.0031101	Paxs	274.97	Joback Method
dvisc	0.0015551	Paxs	314.38	Joback Method
dvisc	0.0009074	Paxs	353.78	Joback Method
dvisc	0.0005898	Paxs	393.19	Joback Method
dvisc	0.0004147	Paxs	432.59	Joback Method
dvisc	0.0003092	Paxs	472.00	Joback Method
dvisc	0.0002413	Paxs	511.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54789309&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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