1-Chloromethyl-3-(1,1-dimethylethyl)benzene

Other names: Benzene,1-(chloromethyl)-3-dimethylethyl)-
Inchi: InChI=1S/C11H15Cl/c1-11(2,3)10-6-4-5-9(7-10)8-12/h4-7H,8H2,1-3H3
InchiKey: QZWCABOLGIVZCP-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: CC(C)(C)c1cccc(CCl)c1
Mol. weight [g/mol]: 182.69
CAS: 38580-79-9

Physical Properties

Property code	Value	Unit	Source
gf	135.43	kJ/mol	Joback Method
hf	-69.80	kJ/mol	Joback Method
hfus	14.68	kJ/mol	Joback Method
hvap	46.11	kJ/mol	Joback Method
ie	8.71 ± 0.03	eV	NIST Webbook
log10ws	-3.82		Crippen Method
logp	3.723		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
tb	516.94	K	Joback Method
tc	739.16	K	Joback Method
tf	285.01	K	Joback Method
vc	0.582	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.36	J/mol×K	516.94	Joback Method
cpg	349.41	J/mol×K	553.98	Joback Method
cpg	364.38	J/mol×K	591.01	Joback Method
cpg	378.31	J/mol×K	628.05	Joback Method
cpg	391.28	J/mol×K	665.09	Joback Method
cpg	403.35	J/mol×K	702.12	Joback Method
cpg	414.58	J/mol×K	739.16	Joback Method

dvisc	0.0032297	Pa×s	285.01	Joback Method
dvisc	0.0015576	Pa×s	323.67	Joback Method
dvisc	0.0008777	Pa×s	362.32	Joback Method
dvisc	0.0005524	Pa×s	400.98	Joback Method
dvisc	0.0003772	Pa×s	439.63	Joback Method
dvisc	0.0002739	Pa×s	478.29	Joback Method
dvisc	0.0002087	Pa×s	516.94	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38580799&Units=SI

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
ie:	Ionization energy
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