Benzene, [1-(chloromethyl)butyl]

Inchi: InChI=1S/C11H15Cl/c1-2-6-11(9-12)10-7-4-3-5-8-10/h3-5,7-8,11H,2,6,9H2,1H3
InchiKey: OMCKNCCLQJXVEQ-UHFFFAOYSA-N
Formula: C11H15Cl
SMILES: CCCC(CCl)c1ccccc1
Mol. weight [g/mol]: 182.69

Physical Properties

Property code	Value	Unit	Source
gf	139.78	kJ/mol	Joback Method
hf	-54.86	kJ/mol	Joback Method
hfus	18.96	kJ/mol	Joback Method
hvap	46.35	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.809		Crippen Method
mcvol	154.330	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
rinpol	1308.00		NIST Webbook
tb	514.75	K	Joback Method
tc	726.81	K	Joback Method
tf	255.07	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	330.19	J/mol×K	514.75	Joback Method
cpg	345.85	J/mol×K	550.09	Joback Method
cpg	360.58	J/mol×K	585.44	Joback Method
cpg	374.40	J/mol×K	620.78	Joback Method
cpg	387.37	J/mol×K	656.12	Joback Method
cpg	399.52	J/mol×K	691.46	Joback Method
cpg	410.90	J/mol×K	726.81	Joback Method
dvisc	0.0049594	Pa×s	255.07	Joback Method
dvisc	0.0020092	Pa×s	298.35	Joback Method

dvisc	0.0010234	Pa×s	341.63	Joback Method
dvisc	0.0006066	Pa×s	384.91	Joback Method
dvisc	0.0003997	Pa×s	428.19	Joback Method
dvisc	0.0002843	Pa×s	471.47	Joback Method
dvisc	0.0002142	Pa×s	514.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R131858&Units=SI
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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume