2-Chloro-6-fluorobenzyl chloride

Other names: Benzene, 1-chloro-2-(chloromethyl)-3-fluoro-
alpha,2-dichloro-6-fluorotoluene
Inchi: InChI=1S/C7H5Cl2F/c8-4-5-6(9)2-1-3-7(5)10/h1-3H,4H2
InchiKey: MJGOLNNLNQQIHR-UHFFFAOYSA-N
Formula: C7H5Cl2F
SMILES: Fc1cccc(Cl)c1CCl
Mol. weight [g/mol]: 179.02
CAS: 55117-15-2

Physical Properties

Property code	Value	Unit	Source
gf	-117.46	kJ/mol	Joback Method
hf	-201.81	kJ/mol	Joback Method
hfus	18.62	kJ/mol	Joback Method
hvap	42.73	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	3.218		Crippen Method
mcvol	111.980	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	470.33	K	Joback Method
tc	687.31	K	Joback Method
tf	280.54	K	Joback Method
vc	0.435	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.08	J/mol×K	470.33	Joback Method
cpg	203.88	J/mol×K	506.49	Joback Method
cpg	212.14	J/mol×K	542.66	Joback Method
cpg	219.90	J/mol×K	578.82	Joback Method
cpg	227.17	J/mol×K	614.98	Joback Method
cpg	233.97	J/mol×K	651.14	Joback Method
cpg	240.32	J/mol×K	687.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C55117152&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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