2-chloro-6-fluorobenzylic alcohol

Other names: 2-Chloro-6-fluorobenzyl alcohol
Inchi: InChI=1S/C7H6ClFO/c8-6-2-1-3-7(9)5(6)4-10/h1-3,10H,4H2
InchiKey: ZZFCUESFXBCRSC-UHFFFAOYSA-N
Formula: C7H6ClFO
SMILES: OCc1c(F)cccc1Cl
Mol. weight [g/mol]: 160.57
CAS: 56456-50-9

Physical Properties

Property code	Value	Unit	Source
gf	-242.35	kJ/mol	Joback Method
hf	-338.30	kJ/mol	Joback Method
hfus	18.51	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-2.63		Crippen Method
logp	1.971		Crippen Method
mcvol	105.610	ml/mol	McGowan Method
pc	4010.84	kPa	Joback Method
tb	525.08	K	Joback Method
tc	722.69	K	Joback Method
tf	311.44	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.23	J/mol×K	525.08	Joback Method
cpg	220.10	J/mol×K	558.01	Joback Method
cpg	227.54	J/mol×K	590.95	Joback Method
cpg	234.56	J/mol×K	623.88	Joback Method
cpg	241.17	J/mol×K	656.82	Joback Method
cpg	247.40	J/mol×K	689.75	Joback Method
cpg	253.25	J/mol×K	722.69	Joback Method

Sources

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=C56456509&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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