2-Chloro-6-fluorobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H14ClFO/c1-2-3-7-14-8-9-10(12)5-4-6-11(9)13/h4-6H,2-3,7-8H2,1H3
InchiKey: RXVKSAQLTSSUEF-UHFFFAOYSA-N
Formula: C11H14ClFO
SMILES: CCCCOCc1c(F)cccc1Cl
Mol. weight [g/mol]: 216.68

Physical Properties

Property code	Value	Unit	Source
gf	-176.85	kJ/mol	Joback Method
hf	-400.85	kJ/mol	Joback Method
hfus	25.97	kJ/mol	Joback Method
hvap	49.66	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.796		Crippen Method
mcvol	161.970	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1411.00		NIST Webbook
tb	546.84	K	Joback Method
tc	744.51	K	Joback Method
tf	317.93	K	Joback Method
vc	0.628	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	363.15	J/mol×K	546.84	Joback Method
cpg	376.69	J/mol×K	579.79	Joback Method
cpg	389.57	J/mol×K	612.73	Joback Method
cpg	401.82	J/mol×K	645.68	Joback Method
cpg	413.43	J/mol×K	678.62	Joback Method
cpg	424.43	J/mol×K	711.57	Joback Method
cpg	434.81	J/mol×K	744.51	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378146&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume