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

Inchi: InChI=1S/C12H16ClFO/c1-2-3-4-8-15-9-10-11(13)6-5-7-12(10)14/h5-7H,2-4,8-9H2,1H3
InchiKey: OAYYYMZUPDSBKA-UHFFFAOYSA-N
Formula: C12H16ClFO
SMILES: CCCCCOCc1c(F)cccc1Cl
Mol. weight [g/mol]: 230.71

Physical Properties

Property code	Value	Unit	Source
gf	-168.43	kJ/mol	Joback Method
hf	-421.49	kJ/mol	Joback Method
hfus	28.56	kJ/mol	Joback Method
hvap	51.88	kJ/mol	Joback Method
log10ws	-4.55		Crippen Method
logp	4.186		Crippen Method
mcvol	176.060	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		NIST Webbook
tb	569.72	K	Joback Method
tc	764.74	K	Joback Method
tf	329.20	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.38	J/mol×K	569.72	Joback Method
cpg	424.71	J/mol×K	602.22	Joback Method
cpg	438.34	J/mol×K	634.73	Joback Method
cpg	451.28	J/mol×K	667.23	Joback Method
cpg	463.56	J/mol×K	699.74	Joback Method
cpg	475.17	J/mol×K	732.24	Joback Method
cpg	486.15	J/mol×K	764.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378149&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
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