

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

Inchi:	InChI=1S/C10H12ClFO/c1-2-6-13-7-8-9(11)4-3-5-10(8)12/h3-5H,2,6-7H2,1H3
InchiKey:	DLEVXSPYPYBBQ-UHFFFAOYSA-N
Formula:	C10H12ClFO
SMILES:	CCCOc1c(F)cccc1Cl
Mol. weight [g/mol]:	202.65

Physical Properties

Property code	Value	Unit	Source
gf	-185.27	kJ/mol	Joback Method
hf	-380.21	kJ/mol	Joback Method
hfus	23.38	kJ/mol	Joback Method
hvap	47.43	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	3.406		Crippen Method
mcvol	147.880	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1313.00		NIST Webbook
tb	523.96	K	Joback Method
tc	724.41	K	Joback Method
tf	306.66	K	Joback Method
vc	0.573	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.71	J/mol×K	523.96	Joback Method
cpg	330.34	J/mol×K	557.37	Joback Method
cpg	342.38	J/mol×K	590.78	Joback Method
cpg	353.82	J/mol×K	624.18	Joback Method
cpg	364.67	J/mol×K	657.59	Joback Method
cpg	374.95	J/mol×K	691.00	Joback Method
cpg	384.66	J/mol×K	724.41	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=U378145&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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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

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