

3,4-Difluorobenzyl alcohol, 1-methylpropyl ether

Inchi:	InChI=1S/C11H14F2O/c1-3-8(2)14-7-9-4-5-10(12)11(13)6-9/h4-6,8H,3,7H2,1-2H3
InchiKey:	GRJMJUOYHMBRCC-UHFFFAOYSA-N
Formula:	C11H14F2O
SMILES:	CCC(C)OCc1ccc(F)c(F)c1
Mol. weight [g/mol]:	200.23

Physical Properties

Property code	Value	Unit	Source
gf	-362.17	kJ/mol	Joback Method
hf	-586.50	kJ/mol	Joback Method
hfus	21.33	kJ/mol	Joback Method
hvap	44.07	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.280		Crippen Method
mcvol	151.500	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	1230.00		NIST Webbook
tb	508.24	K	Joback Method
tc	695.64	K	Joback Method
tf	273.60	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.19	J/mol×K	508.24	Joback Method
cpg	357.06	J/mol×K	539.47	Joback Method
cpg	370.31	J/mol×K	570.71	Joback Method
cpg	382.96	J/mol×K	601.94	Joback Method
cpg	395.01	J/mol×K	633.17	Joback Method
cpg	406.48	J/mol×K	664.41	Joback Method
cpg	417.38	J/mol×K	695.64	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=U378175&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
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

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