3,4-Difluorobenzyl alcohol, 2-methylbutyl ether

Inchi: InChI=1S/C12H16F2O/c1-3-9(2)7-15-8-10-4-5-11(13)12(14)6-10/h4-6,9H,3,7-8H2,1-2H3
InchiKey: JAWGJWTXMXVHKQ-UHFFFAOYSA-N
Formula: C12H16F2O
SMILES: CCC(C)COCc1ccc(F)c(F)c1
Mol. weight [g/mol]: 214.25

Physical Properties

Property code	Value	Unit	Source
gf	-353.75	kJ/mol	Joback Method
hf	-607.14	kJ/mol	Joback Method
hfus	23.92	kJ/mol	Joback Method
hvap	46.29	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.527		Crippen Method
mcvol	165.590	ml/mol	McGowan Method
pc	2127.56	kPa	Joback Method
rinpol	1330.00		NIST Webbook
rinpol	1330.00		NIST Webbook
tb	531.12	K	Joback Method
tc	716.43	K	Joback Method
tf	284.87	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.39	J/mol×K	531.12	Joback Method
cpg	404.09	J/mol×K	562.00	Joback Method
cpg	418.13	J/mol×K	592.89	Joback Method
cpg	431.52	J/mol×K	623.77	Joback Method
cpg	444.27	J/mol×K	654.66	Joback Method
cpg	456.40	J/mol×K	685.54	Joback Method
cpg	467.92	J/mol×K	716.43	Joback Method

Sources

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=U378176&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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