2,5-Difluorobenzyl alcohol, isopropyl ether

Inchi: InChI=1S/C10H12F2O/c1-7(2)13-6-8-5-9(11)3-4-10(8)12/h3-5,7H,6H2,1-2H3
InchiKey: PZPQWIFTZBBAEM-UHFFFAOYSA-N
Formula: C10H12F2O
SMILES: CC(C)OCc1cc(F)ccc1F
Mol. weight [g/mol]: 186.20

Physical Properties

Property code	Value	Unit	Source
gf	-370.59	kJ/mol	Joback Method
hf	-565.86	kJ/mol	Joback Method
hfus	18.74	kJ/mol	Joback Method
hvap	41.84	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.890		Crippen Method
mcvol	137.410	ml/mol	McGowan Method
pc	2561.10	kPa	Joback Method
rinpol	1110.00		NIST Webbook
tb	485.36	K	Joback Method
tc	674.91	K	Joback Method
tf	262.33	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	298.90	J/mol×K	485.36	Joback Method
cpg	311.82	J/mol×K	516.95	Joback Method
cpg	324.17	J/mol×K	548.54	Joback Method
cpg	335.97	J/mol×K	580.13	Joback Method
cpg	347.22	J/mol×K	611.73	Joback Method
cpg	357.94	J/mol×K	643.32	Joback Method
cpg	368.12	J/mol×K	674.91	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=U378162&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
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

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