4-Bromo-2,6-difluorobenzyl alcohol, 3-methylbutyl ether

Inchi: InChI=1S/C12H15BrF2O/c1-8(2)3-4-16-7-10-11(14)5-9(13)6-12(10)15/h5-6,8H,3-4,7H2,1

InchiKey: CLROFRBWOACKRB-UHFFFAOYSA-N

Formula: C12H15BrF2O

SMILES: CC(C)CCOCc1c(F)cc(Br)cc1F

Mol. weight [g/mol]: 293.15

Physical Properties

Property code	Value	Unit	Source
gf	-349.06	kJ/mol	Joback Method
hf	-592.28	kJ/mol	Joback Method
hfus	28.82	kJ/mol	Joback Method
hvap	53.39	kJ/mol	Joback Method
log10ws	-5.12		Crippen Method
logp	4.290		Crippen Method
mcvol	183.090	ml/mol	McGowan Method
pc	2237.64	kPa	Joback Method
rinpol	1525.00		NIST Webbook
rinpol	1525.00		NIST Webbook
tb	602.26	K	Joback Method
tc	801.27	K	Joback Method
tf	357.19	K	Joback Method
vc	0.710	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.35	J/mol×K	602.26	Joback Method
cpg	445.96	J/mol×K	635.43	Joback Method
cpg	458.87	J/mol×K	668.60	Joback Method
cpg	471.10	J/mol×K	701.77	Joback Method
cpg	482.67	J/mol×K	734.94	Joback Method
cpg	493.58	J/mol×K	768.10	Joback Method
cpg	503.86	J/mol×K	801.27	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375284&Units=SI

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