4-Bromo-2,6-difluorobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H13BrF2O/c1-7(2)5-15-6-9-10(13)3-8(12)4-11(9)14/h3-4,7H,5-6H2,1-2H3
InchiKey: JBTTZCFMGGHNGT-UHFFFAOYSA-N
Formula: C11H13BrF2O
SMILES: CC(C)COCc1c(F)cc(Br)cc1F
Mol. weight [g/mol]: 279.12

Physical Properties

Property code	Value	Unit	Source
gf	-357.48	kJ/mol	Joback Method
hf	-571.64	kJ/mol	Joback Method
hfus	26.23	kJ/mol	Joback Method
hvap	51.17	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.900		Crippen Method
mcvol	169.000	ml/mol	McGowan Method
pc	2455.60	kPa	Joback Method
rinpol	1413.00		NIST Webbook
rinpol	1413.00		NIST Webbook
tb	579.38	K	Joback Method
tc	781.24	K	Joback Method
tf	345.92	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.36	J/mol×K	579.38	Joback Method
cpg	397.21	J/mol×K	613.02	Joback Method
cpg	409.42	J/mol×K	646.67	Joback Method
cpg	420.98	J/mol×K	680.31	Joback Method
cpg	431.91	J/mol×K	713.95	Joback Method
cpg	442.23	J/mol×K	747.59	Joback Method
cpg	451.94	J/mol×K	781.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375290&Units=SI
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

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