

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

Inchi:	InChI=1S/C12H15BrF2O/c1-3-8(2)6-16-7-10-11(14)4-9(13)5-12(10)15/h4-5,8H,3,6-7H2,1
InchiKey:	NBBSSGYIWFKIEN-UHFFFAOYSA-N
Formula:	C12H15BrF2O
SMILES:	CCC(C)COc1c(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	1518.00		NIST Webbook
rinpol	1518.00		NIST Webbook
tb	602.26	K	Joback Method
tc	801.27	K	Joback Method
tf	357.19	K	Joback Method
vc	0.710	m ³ /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

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375285&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
hvp:	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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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