4-Bromo-2,6-difluorobenzyl alcohol, n-pentyl ether

Inchi: InChI=1S/C12H15BrF2O/c1-2-3-4-5-16-8-10-11(14)6-9(13)7-12(10)15/h6-7H,2-5,8H2,1H

InchiKey: YNUGRBGTACPWQE-UHFFFAOYSA-N

Formula: C12H15BrF2O

SMILES: CCCCCOCc1c(F)cc(Br)cc1F

Mol. weight [g/mol]: 293.15

Physical Properties

Property code	Value	Unit	Source
gf	-346.62	kJ/mol	Joback Method
hf	-587.00	kJ/mol	Joback Method
hfus	32.34	kJ/mol	Joback Method
hvap	53.78	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.434		Crippen Method
mcvol	183.090	ml/mol	McGowan Method
pc	2220.80	kPa	Joback Method
rinpol	1566.00		NIST Webbook
rinpol	1566.00		NIST Webbook
tb	602.70	K	Joback Method
tc	797.96	K	Joback Method
tf	372.19	K	Joback Method
vc	0.716	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.92	J/mol×K	602.70	Joback Method
cpg	445.22	J/mol×K	635.24	Joback Method
cpg	457.87	J/mol×K	667.79	Joback Method
cpg	469.86	J/mol×K	700.33	Joback Method
cpg	481.23	J/mol×K	732.87	Joback Method
cpg	491.97	J/mol×K	765.42	Joback Method
cpg	502.11	J/mol×K	797.96	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=U375282&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

Latest version available from:
https://www.chemeo.com/cid/49-251-9/4-Bromo-2-6-difluorobenzyl-alcohol-n-pentyl-ether.pdf
Generated by Cheméo on 2024-05-08 18:30:51.368293175 +0000 UTC m=+17482300.288870488.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.