2,3,4,5,6-Pentabromobenzyl alcohol, 2-methylbutyl ether

Inchi: InChI=1S/C12H13Br5O/c1-3-6(2)4-18-5-7-8(13)10(15)12(17)11(16)9(7)14/h6H,3-5H2,1-2

InchiKey: SMQMBZTYGZGJEI-UHFFFAOYSA-N

Formula: C12H13Br5O

SMILES: CCC(C)COCc1c(Br)c(Br)c(Br)c(Br)c1Br

Mol. weight [g/mol]: 572.75

Physical Properties

Property code	Value	Unit	Source
gf	78.58	kJ/mol	Joback Method
hf	-117.68	kJ/mol	Joback Method
hfus	43.02	kJ/mol	Joback Method
hvap	82.09	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	7.062		Crippen Method
mcvol	249.550	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
rinpol	2757.00		NIST Webbook
tb	878.32	K	Joback Method
tc	1137.99	K	Joback Method
tf	620.25	K	Joback Method
vc	0.921	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.01	J/mol×K	878.32	Joback Method
cpg	586.61	J/mol×K	1094.71	Joback Method
cpg	578.84	J/mol×K	1051.43	Joback Method
cpg	570.67	J/mol×K	1008.15	Joback Method
cpg	562.03	J/mol×K	964.88	Joback Method
cpg	552.83	J/mol×K	921.60	Joback Method
cpg	594.05	J/mol×K	1137.99	Joback Method
dvisc	0.0000668	Pa×s	878.32	Joback Method
dvisc	0.0000787	Pa×s	835.31	Joback Method

dvisc	0.0000944	Pa×s	792.30	Joback Method
dvisc	0.0001157	Pa×s	749.28	Joback Method
dvisc	0.0001452	Pa×s	706.27	Joback Method
dvisc	0.0001878	Pa×s	663.26	Joback Method
dvisc	0.0002517	Pa×s	620.25	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=U375313&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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