

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

Inchi:	InChI=1S/C10H9Br5O/c1-4(2)16-3-5-6(11)8(13)10(15)9(14)7(5)12/h4H,3H2,1-2H3
InchiKey:	NNSBCOLNALHIIO-UHFFFAOYSA-N
Formula:	C10H9Br5O
SMILES:	CC(C)OCc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]:	544.70

Physical Properties

Property code	Value	Unit	Source
gf	61.74	kJ/mol	Joback Method
hf	-76.40	kJ/mol	Joback Method
hfus	37.84	kJ/mol	Joback Method
hvap	77.64	kJ/mol	Joback Method
log10ws	-8.62		Crippen Method
logp	6.424		Crippen Method
mcvol	221.370	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
rinpol	2559.00		NIST Webbook
tb	832.56	K	Joback Method
tc	1103.67	K	Joback Method
tf	597.71	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	437.19	J/molxK	832.56	Joback Method
cpg	474.52	J/molxK	1058.48	Joback Method
cpg	467.91	J/molxK	1013.30	Joback Method
cpg	460.94	J/molxK	968.11	Joback Method
cpg	453.55	J/molxK	922.93	Joback Method
cpg	445.65	J/molxK	877.74	Joback Method
cpg	480.83	J/molxK	1103.67	Joback Method
dvisc	0.0000899	Paxs	832.56	Joback Method
dvisc	0.0001049	Paxs	793.42	Joback Method

dvisc	0.0001245	Paxs	754.28	Joback Method
dvisc	0.0001504	Paxs	715.13	Joback Method
dvisc	0.0001859	Paxs	675.99	Joback Method
dvisc	0.0002357	Paxs	636.85	Joback Method
dvisc	0.0003084	Paxs	597.71	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375316&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
mccvol:	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

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