2,3,4,5,6-Pentabromobenzyl alcohol, n-butyl ether

Inchi: InChI=1S/C11H11Br5O/c1-2-3-4-17-5-6-7(12)9(14)11(16)10(15)8(6)13/h2-5H2,1H3
InchiKey: NPJCPTABFRGOHJ-UHFFFAOYSA-N
Formula: C11H11Br5O
SMILES: CCCCOCc1c(Br)c(Br)c(Br)c(Br)c1Br
Mol. weight [g/mol]: 558.72

Physical Properties

Property code	Value	Unit	Source
gf	72.60	kJ/mol	Joback Method
hf	-91.76	kJ/mol	Joback Method
hfus	43.95	kJ/mol	Joback Method
hvap	80.25	kJ/mol	Joback Method
log10ws	-8.93		Crippen Method
logp	6.816		Crippen Method
mcvol	235.460	ml/mol	McGowan Method
pc	3501.28	kPa	Joback Method
rinpol	2717.00		NIST Webbook
rinpol	2717.00		NIST Webbook
tb	855.88	K	Joback Method
tc	1116.22	K	Joback Method
tf	623.98	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	488.92	J/mol×K	855.88	Joback Method
cpg	529.27	J/mol×K	1072.83	Joback Method
cpg	522.05	J/mol×K	1029.44	Joback Method
cpg	514.47	J/mol×K	986.05	Joback Method
cpg	506.47	J/mol×K	942.66	Joback Method
cpg	497.97	J/mol×K	899.27	Joback Method
cpg	536.20	J/mol×K	1116.22	Joback Method
dvisc	0.0000847	Pa×s	855.88	Joback Method

dvisc	0.0000981	Pa×s	817.23	Joback Method
dvisc	0.0001154	Pa×s	778.58	Joback Method
dvisc	0.0001381	Pa×s	739.93	Joback Method
dvisc	0.0001684	Pa×s	701.28	Joback Method
dvisc	0.0002103	Pa×s	662.63	Joback Method
dvisc	0.0002699	Pa×s	623.98	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=U375314&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

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