2,3,5-Triiodobenzyl alcohol, 2-methylpropyl ether

Inchi: InChI=1S/C11H13I3O/c1-7(2)5-15-6-8-3-9(12)4-10(13)11(8)14/h3-4,7H,5-6H2,1-2H3
InchiKey: HWUFKKOWMFCHSQ-UHFFFAOYSA-N
Formula: C11H13I3O
SMILES: CC(C)COCc1cc(I)cc(I)c1I
Mol. weight [g/mol]: 541.93

Physical Properties

Property code	Value	Unit	Source
gf	192.18	kJ/mol	Joback Method
hf	24.86	kJ/mol	Joback Method
hfus	28.00	kJ/mol	Joback Method
hvap	74.48	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	4.673		Crippen Method
mcvol	225.420	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	2448.00		NIST Webbook
rinpol	2448.00		NIST Webbook
tb	794.10	K	Joback Method
tc	1083.19	K	Joback Method
tf	459.12	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.01	J/mol×K	794.10	Joback Method
cpg	511.65	J/mol×K	1035.01	Joback Method
cpg	503.42	J/mol×K	986.83	Joback Method
cpg	494.53	J/mol×K	938.65	Joback Method
cpg	484.89	J/mol×K	890.46	Joback Method
cpg	474.42	J/mol×K	842.28	Joback Method
cpg	519.31	J/mol×K	1083.19	Joback Method
dvisc	0.0000931	Pa×s	794.10	Joback Method

dvisc	0.0001176	Pa×s	738.27	Joback Method
dvisc	0.0001543	Pa×s	682.44	Joback Method
dvisc	0.0002125	Pa×s	626.61	Joback Method
dvisc	0.0003115	Pa×s	570.78	Joback Method
dvisc	0.0004964	Pa×s	514.95	Joback Method
dvisc	0.0008857	Pa×s	459.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375239&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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