

2,3,5-Triiodobenzyl alcohol, 1-methylpropyl ether

Inchi:	InChI=1S/C11H13I3O/c1-3-7(2)15-6-8-4-9(12)5-10(13)11(8)14/h4-5,7H,3,6H2,1-2H3
InchiKey:	RXTSACVWNZKFKZ-UHFFFAOYSA-N
Formula:	C11H13I3O
SMILES:	CCC(C)OCc1cc(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	-6.67		Crippen Method
logp	4.816		Crippen Method
mvol	225.420	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	2438.00		NIST Webbook
tb	794.10	K	Joback Method
tc	1083.19	K	Joback Method
tf	459.12	K	Joback Method
vc	0.820	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	463.01	J/molxK	794.10	Joback Method
cpg	474.42	J/molxK	842.28	Joback Method
cpg	484.89	J/molxK	890.46	Joback Method
cpg	494.53	J/molxK	938.65	Joback Method
cpg	503.42	J/molxK	986.83	Joback Method
cpg	511.65	J/molxK	1035.01	Joback Method
cpg	519.31	J/molxK	1083.19	Joback Method
dvisc	0.0008857	Paxs	459.12	Joback Method
dvisc	0.0004964	Paxs	514.95	Joback Method

dvisc	0.0003115	Paxs	570.78	Joback Method
dvisc	0.0002125	Paxs	626.61	Joback Method
dvisc	0.0001543	Paxs	682.44	Joback Method
dvisc	0.0001176	Paxs	738.27	Joback Method
dvisc	0.0000931	Paxs	794.10	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375236&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

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