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

Inchi: InChI=1S/C12H15I3O/c1-8(2)3-4-16-7-9-5-10(13)6-11(14)12(9)15/h5-6,8H,3-4,7H2,1-2H

InchiKey: VUHFDIODWHOJHV-UHFFFAOYSA-N

Formula: C12H15I3O

SMILES: CC(C)CCOCc1cc(I)cc(I)c1I

Mol. weight [g/mol]: 555.96

Physical Properties

Property code	Value	Unit	Source
gf	200.60	kJ/mol	Joback Method
hf	4.22	kJ/mol	Joback Method
hfus	30.59	kJ/mol	Joback Method
hvap	76.71	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.063		Crippen Method
mcvol	239.510	ml/mol	McGowan Method
pc	2145.33	kPa	Joback Method
rinpol	2567.00		NIST Webbook
rinpol	2567.00		NIST Webbook
tb	816.98	K	Joback Method
tc	1098.55	K	Joback Method
tf	470.39	K	Joback Method
vc	0.875	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	515.43	J/mol×K	816.98	Joback Method
cpg	567.03	J/mol×K	1051.62	Joback Method
cpg	558.24	J/mol×K	1004.69	Joback Method
cpg	548.77	J/mol×K	957.76	Joback Method
cpg	538.55	J/mol×K	910.84	Joback Method
cpg	527.46	J/mol×K	863.91	Joback Method
cpg	575.23	J/mol×K	1098.55	Joback Method
dvisc	0.0000805	Pa×s	816.98	Joback Method

dvisc	0.0001021	Pa×s	759.22	Joback Method
dvisc	0.0001346	Pa×s	701.45	Joback Method
dvisc	0.0001864	Pa×s	643.68	Joback Method
dvisc	0.0002753	Pa×s	585.92	Joback Method
dvisc	0.0004428	Pa×s	528.15	Joback Method
dvisc	0.0008004	Pa×s	470.39	Joback Method

Sources

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=U375234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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