2,3,5-Triiodobenzyl alcohol, neopentyl ether

Inchi: InChI=1S/C12H15I3O/c1-12(2,3)7-16-6-8-4-9(13)5-10(14)11(8)15/h4-5H,6-7H2,1-3H3
InchiKey: BIVLTHOMYUYGJA-UHFFFAOYSA-N
Formula: C12H15I3O
SMILES: CC(C)(C)COCc1cc(I)cc(I)c1I
Mol. weight [g/mol]: 555.96

Physical Properties

Property code	Value	Unit	Source
gf	205.88	kJ/mol	Joback Method
hf	0.75	kJ/mol	Joback Method
hfus	26.70	kJ/mol	Joback Method
hvap	75.80	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	5.063		Crippen Method
mcvol	239.510	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	2466.00		NIST Webbook
rinpol	2466.00		NIST Webbook
tb	814.19	K	Joback Method
tc	1106.78	K	Joback Method
tf	487.81	K	Joback Method
vc	0.871	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.84	J/mol×K	814.19	Joback Method
cpg	528.90	J/mol×K	862.96	Joback Method
cpg	540.01	J/mol×K	911.72	Joback Method
cpg	550.35	J/mol×K	960.49	Joback Method
cpg	560.05	J/mol×K	1009.25	Joback Method
cpg	569.28	J/mol×K	1058.02	Joback Method
cpg	578.18	J/mol×K	1106.78	Joback Method
dvisc	0.0006701	Pa×s	487.81	Joback Method

dvisc	0.0003807	Pa×s	542.21	Joback Method
dvisc	0.0002398	Pa×s	596.60	Joback Method
dvisc	0.0001632	Pa×s	651.00	Joback Method
dvisc	0.0001178	Pa×s	705.40	Joback Method
dvisc	0.0000891	Pa×s	759.79	Joback Method
dvisc	0.0000700	Pa×s	814.19	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U375231&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