

4-Benzyloxyiodobenzene

Inchi:	InChI=1S/C13H11IO/c14-12-6-8-13(9-7-12)15-10-11-4-2-1-3-5-11/h1-9H,10H2
InchiKey:	MPWFGAWFTAZWKZ-UHFFFAOYSA-N
Formula:	C13H11IO
SMILES:	Ic1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	310.13
CAS:	19578-68-8

Physical Properties

Property code	Value	Unit	Source
gf	226.89	kJ/mol	Joback Method
hf	94.59	kJ/mol	Joback Method
hfus	22.71	kJ/mol	Joback Method
hvap	61.53	kJ/mol	Joback Method
log10ws	-4.85		Crippen Method
logp	3.870		Crippen Method
mcvol	178.200	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
tb	670.74	K	Joback Method
tc	941.68	K	Joback Method
tf	381.92	K	Joback Method
vc	0.653	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	398.31	J/molxK	670.74	Joback Method
cpg	412.77	J/molxK	715.90	Joback Method
cpg	425.95	J/molxK	761.05	Joback Method
cpg	437.91	J/molxK	806.21	Joback Method
cpg	448.75	J/molxK	851.36	Joback Method
cpg	458.56	J/molxK	896.52	Joback Method
cpg	467.42	J/molxK	941.68	Joback Method
dvisc	0.0014344	Paxs	381.92	Joback Method
dvisc	0.0007918	Paxs	430.06	Joback Method

dvisc	0.0004926	Paxs	478.19	Joback Method
dvisc	0.0003342	Paxs	526.33	Joback Method
dvisc	0.0002420	Paxs	574.47	Joback Method
dvisc	0.0001842	Paxs	622.60	Joback Method
dvisc	0.0001458	Paxs	670.74	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C19578688&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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