Benzene, 1-iodo-4-(2-phenylethyl)-

Other names: Bibenzyl, 4-iodo-
1-Iodo-4-(2-phenylethyl)benzene
1-(4-Iodophenyl)-2-phenylethane
Inchi: InChI=1S/C14H13I/c15-14-10-8-13(9-11-14)7-6-12-4-2-1-3-5-12/h1-5,8-11H,6-7H2
InchiKey: CTNREHGTRZZBQM-UHFFFAOYSA-N
Formula: C14H13I
SMILES: Ic1ccc(CCc2ccccc2)cc1
Mol. weight [g/mol]: 308.16
CAS: 14310-25-9

Physical Properties

Property code	Value	Unit	Source
gf	340.31	kJ/mol	Joback Method
hf	206.17	kJ/mol	Joback Method
hfus	24.11	kJ/mol	Joback Method
hvap	61.34	kJ/mol	Joback Method
ie	8.70 ± 0.10	eV	NIST Webbook
log10ws	-5.04		Crippen Method
logp	4.076		Crippen Method
mcvol	186.420	ml/mol	McGowan Method
pc	2665.27	kPa	Joback Method
tb	671.20	K	Joback Method
tc	940.53	K	Joback Method
tf	370.96	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.89	J/mol×K	671.20	Joback Method
cpg	488.91	J/mol×K	895.65	Joback Method
cpg	478.15	J/mol×K	850.76	Joback Method
cpg	466.40	J/mol×K	805.87	Joback Method
cpg	453.52	J/mol×K	760.98	Joback Method

cpg	439.39	J/mol×K	716.09	Joback Method
cpg	498.77	J/mol×K	940.53	Joback Method
dvisc	0.0001672	Pa×s	671.20	Joback Method
dvisc	0.0002126	Pa×s	621.16	Joback Method
dvisc	0.0002819	Pa×s	571.12	Joback Method
dvisc	0.0003945	Pa×s	521.08	Joback Method
dvisc	0.0005931	Pa×s	471.04	Joback Method
dvisc	0.0009824	Pa×s	421.00	Joback Method
dvisc	0.0018644	Pa×s	370.96	Joback Method

Sources

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=C14310259&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ie: Ionization energy
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