Bicyclo[2.2.2]octane, 1-iodo-

Other names: 1-Iodobicyclo[2.2.2]octane
Inchi: InChI=1S/C8H13I/c9-8-4-1-7(2-5-8)3-6-8/h7H,1-6H2
InchiKey: SMDJHIPXLFNPTJ-UHFFFAOYSA-N
Formula: C8H13I
SMILES: IC12CCC(CC1)CC2
Mol. weight [g/mol]: 236.09
CAS: 931-98-6

Physical Properties

Property code	Value	Unit	Source
gf	166.41	kJ/mol	Joback Method
hf	16.94	kJ/mol	Joback Method
hfus	6.65	kJ/mol	Joback Method
hvap	41.79	kJ/mol	Joback Method
ie	8.87	eV	NIST Webbook
ie	8.70	eV	NIST Webbook
log10ws	-3.78		Crippen Method
logp	3.144		Crippen Method
mcvol	127.680	ml/mol	McGowan Method
pc	3659.77	kPa	Joback Method
tb	497.84	K	Joback Method
tc	757.33	K	Joback Method
tf	290.72	K	Joback Method
vc	0.468	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.16	J/mol×K	497.84	Joback Method
cpg	278.67	J/mol×K	541.09	Joback Method
cpg	294.46	J/mol×K	584.34	Joback Method
cpg	308.78	J/mol×K	627.58	Joback Method
cpg	321.92	J/mol×K	670.83	Joback Method
cpg	334.15	J/mol×K	714.08	Joback Method

cpg	345.73	J/mol×K	757.33	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=C931986&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
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