Bicyclo[2.2.1]heptane, 1-iodo-

Other names: 1-Iodobicyclo[2.2.1]heptane
Inchi: InChI=1S/C7H11I/c8-7-3-1-6(5-7)2-4-7/h6H,1-5H2
InchiKey: USKGOFKHICIEEW-UHFFFAOYSA-N
Formula: C7H11I
SMILES: IC12CCC(CC1)C2
Mol. weight [g/mol]: 222.07
CAS: 930-80-3

Physical Properties

Property code	Value	Unit	Source
gf	170.09	kJ/mol	Joback Method
hf	43.74	kJ/mol	Joback Method
hfus	6.16	kJ/mol	Joback Method
hvap	39.40	kJ/mol	Joback Method
ie	8.80	eV	NIST Webbook
ie	8.96	eV	NIST Webbook
log10ws	-3.36		Crippen Method
logp	2.754		Crippen Method
mcvol	113.590	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	470.69	K	Joback Method
tc	724.94	K	Joback Method
tf	282.97	K	Joback Method
vc	0.419	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.64	J/mol×K	470.69	Joback Method
cpg	234.29	J/mol×K	513.07	Joback Method
cpg	248.24	J/mol×K	555.44	Joback Method
cpg	260.75	J/mol×K	597.82	Joback Method
cpg	272.08	J/mol×K	640.19	Joback Method
cpg	282.51	J/mol×K	682.57	Joback Method

cpg	292.29	J/mol×K	724.94	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=C930803&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
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