

Bicyclo[2.2.1]heptane, 2-iodo-, endo-

Inchi:	InChI=1S/C7H11I/c8-7-4-5-1-2-6(7)3-5/h5-7H,1-4H2/t5?,6?,7-/m0/s1
InchiKey:	IUXVGOYYSBDCSW-AHXFUIDQSA-N
Formula:	C7H11I
SMILES:	IC1CC2CCC1C2
Mol. weight [g/mol]:	222.07
CAS:	57173-48-5

Physical Properties

Property code	Value	Unit	Source
gf	167.87	kJ/mol	Joback Method
hf	8.16	kJ/mol	Joback Method
hfus	13.53	kJ/mol	Joback Method
hvap	40.24	kJ/mol	Joback Method
ie	9.00	eV	NIST Webbook
log10ws	-3.12		Crippen Method
logp	2.610		Crippen Method
mcvol	113.590	ml/mol	McGowan Method
pc	3628.97	kPa	Joback Method
tb	465.78	K	Joback Method
tc	708.38	K	Joback Method
tf	254.83	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.93	J/molxK	465.78	Joback Method
cpg	287.38	J/molxK	667.95	Joback Method
cpg	275.87	J/molxK	627.52	Joback Method
cpg	263.36	J/molxK	587.08	Joback Method
cpg	249.77	J/molxK	546.65	Joback Method
cpg	234.99	J/molxK	506.21	Joback Method
cpg	298.01	J/molxK	708.38	Joback Method
dvisc	0.0010018	Paxs	465.78	Joback Method

dvisc	0.0010483	Paxs	430.62	Joback Method
dvisc	0.0011059	Paxs	395.46	Joback Method
dvisc	0.0011788	Paxs	360.30	Joback Method
dvisc	0.0012741	Paxs	325.15	Joback Method
dvisc	0.0014033	Paxs	289.99	Joback Method
dvisc	0.0015873	Paxs	254.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C57173485&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
log_p:	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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