

Cyclohexene, 1-iodo-6-methyl-

Inchi:	InChI=1S/C7H11I/c1-6-4-2-3-5-7(6)8/h5-6H,2-4H2,1H3
InchiKey:	ZDARRRISQKLIU-UHFFFAOYSA-N
Formula:	C7H11I
SMILES:	CC1CCCC=C1I
Mol. weight [g/mol]:	222.07
CAS:	40648-10-0

Physical Properties

Property code	Value	Unit	Source
gf	110.96	kJ/mol	Joback Method
hf	-10.31	kJ/mol	Joback Method
hfus	10.96	kJ/mol	Joback Method
hvap	41.93	kJ/mol	Joback Method
log10ws	-3.70		Crippen Method
logp	3.125		Crippen Method
mcvol	120.150	ml/mol	McGowan Method
pc	3517.91	kPa	Joback Method
rinpol	1157.00		NIST Webbook
tb	476.39	K	Joback Method
tc	722.59	K	Joback Method
tf	247.37	K	Joback Method
vc	0.434	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	216.17	J/molxK	476.39	Joback Method
cpg	279.33	J/molxK	681.56	Joback Method
cpg	268.44	J/molxK	640.53	Joback Method
cpg	256.72	J/molxK	599.49	Joback Method
cpg	244.12	J/molxK	558.46	Joback Method
cpg	230.62	J/molxK	517.42	Joback Method
cpg	289.44	J/molxK	722.59	Joback Method
dvisc	0.0003557	Paxs	476.39	Joback Method

dvisc	0.0004513	Paxs	438.22	Joback Method
dvisc	0.0005992	Paxs	400.05	Joback Method
dvisc	0.0008447	Paxs	361.88	Joback Method
dvisc	0.0012912	Paxs	323.71	Joback Method
dvisc	0.0022107	Paxs	285.54	Joback Method
dvisc	0.0044685	Paxs	247.37	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40648100&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
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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