

3-Iodo-2-butanone

Inchi:	InChI=1S/C4H7IO/c1-3(5)4(2)6/h3H,1-2H3
InchiKey:	FPEIUGALYUCCPS-UHFFFAOYSA-N
Formula:	C4H7IO
SMILES:	CC(=O)C(C)I
Mol. weight [g/mol]:	198.00
CAS:	30719-18-7

Physical Properties

Property code	Value	Unit	Source
gf	-90.44	kJ/mol	Joback Method
hf	-160.00 ± 3.00	kJ/mol	NIST Webbook
hf	-160.00 ± 3.00	kJ/mol	NIST Webbook
hfus	8.60	kJ/mol	Joback Method
hvap	40.23	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.399		Crippen Method
mcvol	94.610	ml/mol	McGowan Method
pc	4146.27	kPa	Joback Method
tb	437.49	K	Joback Method
tc	660.58	K	Joback Method
tf	227.83	K	Joback Method
vc	0.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.82	J/mol×K	437.49	Joback Method
cpg	181.69	J/mol×K	623.40	Joback Method
cpg	175.74	J/mol×K	586.22	Joback Method
cpg	169.41	J/mol×K	549.04	Joback Method
cpg	162.65	J/mol×K	511.85	Joback Method
cpg	155.47	J/mol×K	474.67	Joback Method
cpg	187.26	J/mol×K	660.58	Joback Method
dvisc	0.0004498	Paxs	437.49	Joback Method

dvisc	0.0005853	Paxs	402.55	Joback Method
dvisc	0.0008006	Paxs	367.60	Joback Method
dvisc	0.0011696	Paxs	332.66	Joback Method
dvisc	0.0018676	Paxs	297.72	Joback Method
dvisc	0.0033776	Paxs	262.77	Joback Method
dvisc	0.0073258	Paxs	227.83	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C30719187&Units=SI

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
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

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