Acetyl iodide

Other names: UN 1898
Inchi: InChI=1S/C2H3IO/c1-2(3)4/h1H3
InchiKey: LEKJTGQWLAUGQA-UHFFFAOYSA-N
Formula: C2H3IO
SMILES: CC(=O)I
Mol. weight [g/mol]: 169.95
CAS: 507-02-8

Physical Properties

Property code	Value	Unit	Source
gf	-104.84	kJ/mol	Joback Method
hf	-127.00 ± 2.00	kJ/mol	NIST Webbook
hf	-133.00	kJ/mol	NIST Webbook
hf	-125.00 ± 3.60	kJ/mol	NIST Webbook
hfl	-162.30 ± 0.88	kJ/mol	NIST Webbook
hfl	-166.30 ± 0.20	kJ/mol	NIST Webbook
hfl	-166.30 ± 0.30	kJ/mol	NIST Webbook
hfus	6.94	kJ/mol	Joback Method
hvap	33.00	kJ/mol	NIST Webbook
hvap	38.50 ± 3.30	kJ/mol	NIST Webbook
log10ws	-1.38		Crippen Method
logp	0.968		Crippen Method
mcvol	66.430	ml/mol	McGowan Method
pc	5335.72	kPa	Joback Method
tb	381.20	K	NIST Webbook
tb	378.00 ± 3.00	K	NIST Webbook
tb	381.00	K	NIST Webbook
tb	381.00	K	NIST Webbook
tc	615.29	K	Joback Method
tf	220.29	K	Joback Method
vc	0.241	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	80.35	J/mol×K	392.17	Joback Method
cpg	84.27	J/mol×K	429.36	Joback Method
cpg	87.94	J/mol×K	466.54	Joback Method
cpg	91.37	J/mol×K	503.73	Joback Method
cpg	94.57	J/mol×K	540.92	Joback Method
cpg	97.56	J/mol×K	578.11	Joback Method
cpg	100.35	J/mol×K	615.29	Joback Method
dvisc	0.0046802	Pa×s	220.29	Joback Method
dvisc	0.0026341	Pa×s	248.94	Joback Method
dvisc	0.0016692	Pa×s	277.58	Joback Method
dvisc	0.0011520	Pa×s	306.23	Joback Method
dvisc	0.0008472	Pa×s	334.88	Joback Method
dvisc	0.0006539	Pa×s	363.52	Joback Method
dvisc	0.0005242	Pa×s	392.17	Joback Method
hvapt	37.10	kJ/mol	289.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	309.20	K	6.70	NIST Webbook
tbrp	309.00	K	6.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.14626e+01
Coeff. B	-8.50106e+03
Coeff. C	1.23536e+02
Temperature range (K), min.	272.55
Temperature range (K), max.	402.81

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C507028&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume