Acetyl bromide

Other names:	CH3COBr
	UN 1716
Inchi:	InChI=1S/C2H3BrO/c1-2(3)4/h1H3
InchiKey:	FXXACINHVKSMDR-UHFFFAOYSA-N
Formula:	C2H3BrO
SMILES:	CC(=O)Br
Mol. weight [g/mol]:	122.95
CAS:	506-96-7

Physical Properties

Property code	Value	Unit	Source
gf	-148.64	kJ/mol	Joback Method
hf	-195.00	kJ/mol	NIST Webbook
hf	-196.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-223.30 ± 0.63	kJ/mol	NIST Webbook
hfl	-226.00 ± 0.54	kJ/mol	NIST Webbook
hfus	7.82	kJ/mol	Joback Method
hvap	31.00	kJ/mol	NIST Webbook
hvap	29.60 ± 0.30	kJ/mol	NIST Webbook
ie	10.55 ± 0.05	eV	NIST Webbook
ie	10.24	eV	NIST Webbook
ie	10.68 ± 0.05	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.928		Crippen Method
mcvol	58.110	ml/mol	McGowan Method
pc	6122.63	kPa	Joback Method
tb	349.00 ± 3.00	K	NIST Webbook
tb	353.65 ± 1.50	K	NIST Webbook
tb	349.20	K	NIST Webbook
tb	349.07 ± 0.50	K	NIST Webbook
tb	349.85 ± 0.50	K	NIST Webbook
tc	568.09	K	Joback Method
tf	176.65 ± 0.50	K	NIST Webbook
tf	177.00	K	NIST Webbook
vc	0.215	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.06	J/mol×K	534.28	Joback Method
cpg	85.67	J/mol×K	466.64	Joback Method
cpg	82.18	J/mol×K	432.82	Joback Method
cpg	78.50	J/mol×K	399.01	Joback Method
cpg	74.60	J/mol×K	365.19	Joback Method
cpg	88.96	J/mol×K	500.46	Joback Method
cpg	94.99	J/mol×K	568.09	Joback Method
dvisc	0.0028529	Pa×s	222.03	Joback Method
dvisc	0.0004631	Pa×s	365.19	Joback Method
dvisc	0.0005640	Pa×s	341.33	Joback Method
dvisc	0.0007076	Pa×s	317.47	Joback Method
dvisc	0.0009210	Pa×s	293.61	Joback Method
dvisc	0.0012559	Pa×s	269.75	Joback Method
dvisc	0.0018190	Pa×s	245.89	Joback Method
hvapt	30.30	kJ/mol	348.10	NIST Webbook
hvapt	29.50	kJ/mol	311.50	NIST Webbook
hvapt	31.40	kJ/mol	304.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	344.00	K	100.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.08477e+01
Coeff. B	-1.47780e+03
Coeff. C	-1.11920e+02
Temperature range (K), min.	251.86

Temperature range (K), max.	378.85

Sources

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=C506967&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

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
ie:	Ionization energy
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