

Acetyl bromide

Other names:	CH ₃ COBr UN 1716
Inchi:	InChI=1S/C2H3BrO/c1-2(3)4/h1H3
InchiKey:	FXXACINHVKSMR-UHFFFAOYSA-N
Formula:	C ₂ H ₃ BrO
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	-196.00 ± 3.00	kJ/mol	NIST Webbook
hf	-195.00	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	29.60 ± 0.30	kJ/mol	NIST Webbook
hvap	31.00	kJ/mol	NIST Webbook
ie	10.55 ± 0.05	eV	NIST Webbook
ie	10.68 ± 0.05	eV	NIST Webbook
ie	10.24	eV	NIST Webbook
log10ws	-0.87		Crippen Method
logp	0.928		Crippen Method
mvol	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	349.07 ± 0.50	K	NIST Webbook
tb	349.20	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	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	88.96	J/molxK	500.46	Joback Method
cpg	94.99	J/molxK	568.09	Joback Method
cpg	92.06	J/molxK	534.28	Joback Method
cpg	74.60	J/molxK	365.19	Joback Method
cpg	78.50	J/molxK	399.01	Joback Method
cpg	82.18	J/molxK	432.82	Joback Method
cpg	85.67	J/molxK	466.64	Joback Method
dvisc	0.0004631	Paxs	365.19	Joback Method
dvisc	0.0007076	Paxs	317.47	Joback Method
dvisc	0.0005640	Paxs	341.33	Joback Method
dvisc	0.0028529	Paxs	222.03	Joback Method
dvisc	0.0018190	Paxs	245.89	Joback Method
dvisc	0.0012559	Paxs	269.75	Joback Method
dvisc	0.0009210	Paxs	293.61	Joback Method
hvapt	30.30	kJ/mol	348.10	NIST Webbook
hvapt	31.40	kJ/mol	304.00	NIST Webbook
hvapt	29.50	kJ/mol	311.50	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	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.08477e+01
Coeff. B	-1.47780e+03
Coeff. C	-1.11920e+02
Temperature range (K), min.	251.86

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/ci9903071

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

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