

2,3-Butanedione

Other names:	Biacetyl Butane-2,3-dione Butanedione Diacetyl Dimethyl diketone Dimethyl glyoxal 2,3-Butadione 2,3-Diketobutane (CH ₃ CO) ₂ Glyoxal, dimethyl- Butadione UN 2346 2,3-Dioxobutane 2,3-Butandione Buta-2,3-dione Butan-2,3-dione NSC 8750 butane-2,3-dione (diacetyl) 2,3-butanedione (diacetal) 2,3-butanedione (diacetyl) Butan-2,3-dione (diacetyl) Butanedione (diacetyl) 2,3 Butandione (Diacetyl) 2,3-butanodione
Inchi:	InChI=1S/C4H6O2/c1-3(5)4(2)6/h1-2H3
InchiKey:	QSJXEFYPDANLFS-UHFFFAOYSA-N
Formula:	C ₄ H ₆ O ₂
SMILES:	CC(=O)C(C)=O
Mol. weight [g/mol]:	86.09
CAS:	431-03-8

Physical Properties

Property code	Value	Unit	Source
affp	801.90	kJ/mol	NIST Webbook
basg	770.10	kJ/mol	NIST Webbook
chl	-2066.10 ± 0.79	kJ/mol	NIST Webbook

ea	0.69 ± 0.10	eV	NIST Webbook
ea	1.10	eV	NIST Webbook
gf	-275.04	kJ/mol	Joback Method
hf	-326.80	kJ/mol	NIST Webbook
hfl	-365.50	kJ/mol	NIST Webbook
hfus	9.31	kJ/mol	Joback Method
hvap	38.70 ± 0.92	kJ/mol	NIST Webbook
ie	9.57 ± 0.05	eV	NIST Webbook
ie	9.60	eV	NIST Webbook
ie	9.23 ± 0.03	eV	NIST Webbook
ie	9.56	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
ie	9.72	eV	NIST Webbook
ie	9.47	eV	NIST Webbook
ie	9.30	eV	NIST Webbook
ie	9.25 ± 0.03	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
log10ws	-0.06		Crippen Method
logp	0.164		Crippen Method
mcvol	70.360	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
rinpol	590.00		NIST Webbook
rinpol	558.00		NIST Webbook
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tf	234.70	K	Joback Method
vc	0.272	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	151.66	J/molxK	559.57	Joback Method
cpg	146.06	J/molxK	527.39	Joback Method
cpg	140.19	J/molxK	495.21	Joback Method
cpg	134.06	J/molxK	463.02	Joback Method
cpg	127.65	J/molxK	430.84	Joback Method
cpg	120.97	J/molxK	398.66	Joback Method
cpg	157.00	J/molxK	591.75	Joback Method
dvisc	0.0028535	Paxs	234.70	Joback Method
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Sources

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Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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