2,3-Butanedione

Inchi: InChI=1S/C4H6O2/c1-3(5)4(2)6/h1-2H3
InchiKey: QSJXEFYPDANLFS-UHFFFAOYSA-N
Formula: C4H6O2
SMILES: CC(=O)C(C)=O
Mol. weight [g/mol]: 86.09
CAS: 625-34-3

Physical Properties

Property code	Value	Unit	Source
chl	-2066.10 ± 0.79	kJ/mol	NIST Webbook
chl	-2107.00	kJ/mol	NIST Webbook
chl	-2070.00 ± 0.80	kJ/mol	NIST Webbook
chl	-2065.10	kJ/mol	NIST Webbook
gf	-275.04	kJ/mol	Joback Method
hf	-326.80	kJ/mol	NIST Webbook
hfl	-337.00	kJ/mol	NIST Webbook
hfl	-361.00	kJ/mol	NIST Webbook
hfl	-366.50 ± 0.84	kJ/mol	NIST Webbook
hfl	-365.50	kJ/mol	NIST Webbook
hfus	9.31	kJ/mol	Joback Method
hvap	36.00	kJ/mol	NIST Webbook
hvap	38.70 ± 0.92	kJ/mol	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
tb	398.66	K	Joback Method
tc	591.75	K	Joback Method
tf	234.70	K	Joback Method
vc	0.272	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	120.97	J/mol×K	398.66	Joback Method
cpg	151.66	J/mol×K	559.57	Joback Method
cpg	146.06	J/mol×K	527.39	Joback Method
cpg	140.19	J/mol×K	495.21	Joback Method
cpg	134.06	J/mol×K	463.02	Joback Method
cpg	127.65	J/mol×K	430.84	Joback Method
cpg	157.00	J/mol×K	591.75	Joback Method
dvisc	0.0003612	Pa×s	398.66	Joback Method
dvisc	0.0004491	Pa×s	371.33	Joback Method
dvisc	0.0005780	Pa×s	344.01	Joback Method
dvisc	0.0007769	Pa×s	316.68	Joback Method
dvisc	0.0011044	Pa×s	289.35	Joback Method
dvisc	0.0016895	Pa×s	262.03	Joback Method
dvisc	0.0028535	Pa×s	234.70	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C625343&Units=SI

Legend

chl: Standard liquid enthalpy of combustion
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
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