2,4-Hexanedione

Other names: Acetone, propionyl-
Hexane-2,4-dione
Propionylacetone
Inchi: InChI=1S/C6H10O2/c1-3-6(8)4-5(2)7/h3-4H2,1-2H3
InchiKey: NDOGLIPWGGRQCO-UHFFFAOYSA-N
Formula: C6H10O2
SMILES: CCC(=O)CC(C)=O
Mol. weight [g/mol]: 114.14
CAS: 3002-24-2

Physical Properties

Property code	Value	Unit	Source
chl	-3281.00 ± 6.30	kJ/mol	NIST Webbook
gf	-258.20	kJ/mol	Joback Method
hf	-439.70	kJ/mol	NIST Webbook
hfl	-505.00 ± 3.00	kJ/mol	NIST Webbook
hfus	14.49	kJ/mol	Joback Method
hvap	23.00 ± 0.30	kJ/mol	NIST Webbook
log10ws	-0.89		Crippen Method
logp	0.945		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	892.19		NIST Webbook
rinpol	895.93		NIST Webbook
rinpol	880.00		NIST Webbook
rinpol	885.00		NIST Webbook
rinpol	862.00		NIST Webbook
rinpol	888.20		NIST Webbook
rinpol	900.00		NIST Webbook
ripol	1209.00		NIST Webbook
tb	431.20	K	NIST Webbook
tc	634.10	K	Joback Method
tf	257.24	K	Joback Method
vc	0.384	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.61	J/mol×K	444.42	Joback Method
cpg	237.09	J/mol×K	602.49	Joback Method
cpg	229.18	J/mol×K	570.87	Joback Method
cpg	220.89	J/mol×K	539.26	Joback Method
cpg	212.20	J/mol×K	507.65	Joback Method
cpg	203.11	J/mol×K	476.03	Joback Method
cpg	244.62	J/mol×K	634.10	Joback Method
dvisc	0.0003624	Pa×s	444.42	Joback Method
dvisc	0.0004571	Pa×s	413.22	Joback Method
dvisc	0.0005990	Pa×s	382.03	Joback Method
dvisc	0.0008236	Pa×s	350.83	Joback Method
dvisc	0.0012049	Pa×s	319.63	Joback Method
dvisc	0.0019141	Pa×s	288.44	Joback Method
dvisc	0.0034020	Pa×s	257.24	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	327.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.51538e+01
Coeff. B	-3.89425e+03
Coeff. C	-6.15660e+01
Temperature range (K), min.	323.52
Temperature range (K), max.	457.23

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3002242&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

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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume