2,5-Hexanedione

Other names:	«alpha»,«beta»-Diacetylethane
	Acetonyl acetone
	Diacetonyl
	1,2-Diacetylethane
	2,5-Hexadione
	Hexane-2,5-dione
	Hexanedione-(2,5)
	Acetone, acetonyl-
	HDO
	2,5-Diketohexane
	CH3COCH2CH2COCH3
	2,5-Dioxohexane
	NSC 7621
Inchi:	InChI=1S/C6H10O2/c1-5(7)3-4-6(2)8/h3-4H2,1-2H3
InchiKey:	OJVAMHKKJGICOG-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CC(=O)CCC(C)=O
Mol. weight [g/mol]:	114.14
CAS:	110-13-4

Physical Properties

Property code	Value	Unit	Source
affp	892.00	kJ/mol	NIST Webbook
basg	851.80	kJ/mol	NIST Webbook
gf	-258.20	kJ/mol	Joback Method
hf	-392.33	kJ/mol	Joback Method
hfus	14.49	kJ/mol	Joback Method
hvap	42.44	kJ/mol	Joback Method
log10ws	-0.89		Crippen Method
logp	0.945		Crippen Method
mcvol	98.540	ml/mol	McGowan Method
pc	3594.25	kPa	Joback Method
rinpol	888.00		NIST Webbook
rinpol	135.50		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	890.00		NIST Webbook

rinpol	890.00		NIST Webbook
rinpol	894.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	906.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	931.00		NIST Webbook
rinpol	932.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	920.00		NIST Webbook
ripol	1485.00		NIST Webbook
ripol	1505.00		NIST Webbook
ripol	1515.00		NIST Webbook
ripol	1500.00		NIST Webbook
ripol	1500.00		NIST Webbook
tb	463.40 ± 1.00	K	NIST Webbook
tb	467.15 ± 2.00	K	NIST Webbook
tb	467.15 ± 3.00	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	244.62	J/mol×K	634.10	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	193.61	J/mol×K	444.42	Joback Method
dvisc	0.0034020	Pa×s	257.24	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
hvapt	50.10	kJ/mol	430.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.70	K	1.30	NIST Webbook

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=C110134&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: 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
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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point

vc: Critical Volume