3,4-Hexanedione

Other names:	3,4-Hexandione
	Bipropionyl
	hexane-3,4-dione
Inchi:	InChI=1S/C6H10O2/c1-3-5(7)6(8)4-2/h3-4H2,1-2H3
InchiKey:	KVFQMAZOBTXCAZ-UHFFFAOYSA-N
Formula:	C6H10O2
SMILES:	CCC(=O)C(=O)CC
Mol. weight [g/mol]:	114.14
CAS:	4437-51-8

Physical Properties

Property code	Value	Unit	Source
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	777.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	773.40		NIST Webbook
rinpol	816.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	804.00		NIST Webbook
rinpol	777.00		NIST Webbook
rinpol	801.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	773.00		NIST Webbook
ripol	1143.00		NIST Webbook
ripol	1183.00		NIST Webbook
ripol	1140.00		NIST Webbook
ripol	1123.00		NIST Webbook
ripol	1151.00		NIST Webbook

ripol	1135.00		NIST Webbook
ripol	1151.00		NIST Webbook
ripol	1157.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1164.00		NIST Webbook
ripol	1143.00		NIST Webbook
ripol	1135.00		NIST Webbook
ripol	1143.00		NIST Webbook
tb	403.20	K	NIST Webbook
tb	397.20	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	203.11	J/mol×K	476.03	Joback Method
cpg	212.20	J/mol×K	507.65	Joback Method
cpg	220.89	J/mol×K	539.26	Joback Method
cpg	229.18	J/mol×K	570.87	Joback Method
cpg	237.09	J/mol×K	602.49	Joback Method
cpg	244.62	J/mol×K	634.10	Joback Method
dvisc	0.0034020	Pa×s	257.24	Joback Method
dvisc	0.0019141	Pa×s	288.44	Joback Method
dvisc	0.0012049	Pa×s	319.63	Joback Method
dvisc	0.0008236	Pa×s	350.83	Joback Method
dvisc	0.0005990	Pa×s	382.03	Joback Method
dvisc	0.0004571	Pa×s	413.22	Joback Method
dvisc	0.0003624	Pa×s	444.42	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55380e+01

Coeff. B	-3.75609e+03
Coeff. C	-5.32260e+01
Temperature range (K), min.	299.52
Temperature range (K), max.	420.51

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4437518&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

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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume