2,4-Octanedione

Other names:	2,4-octadione
	octane-2,4-dione
Inchi:	InChI=1S/C8H14O2/c1-3-4-5-8(10)6-7(2)9/h3-6H2,1-2H3
InchiKey:	GJYXGIIWJFZCLN-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CCCCC(=O)CC(C)=O
Mol. weight [g/mol]:	142.20
CAS:	14090-87-0

Physical Properties

Property code	Value	Unit	Source
gf	-241.36	kJ/mol	Joback Method
hf	-456.90	kJ/mol	NIST Webbook
hfus	19.67	kJ/mol	Joback Method
hvap	46.89	kJ/mol	Joback Method
log10ws	-1.56		Aqueous Solubility Prediction Method
logp	1.725		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	1079.34		NIST Webbook
rinpol	1086.32		NIST Webbook
rinpol	1091.42		NIST Webbook
rinpol	1083.01		NIST Webbook
tb	490.18	K	Joback Method
tc	675.94	K	Joback Method
tf	279.78	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.20	J/mol×K	490.18	Joback Method
cpg	286.97	J/mol×K	521.14	Joback Method

cpg	298.23	J/mol×K	552.10	Joback Method
cpg	308.97	J/mol×K	583.06	Joback Method
cpg	319.22	J/mol×K	614.02	Joback Method
cpg	328.98	J/mol×K	644.98	Joback Method
cpg	338.27	J/mol×K	675.94	Joback Method
dvisc	0.0036359	Pa×s	279.78	Joback Method
dvisc	0.0019569	Pa×s	314.85	Joback Method
dvisc	0.0011925	Pa×s	349.91	Joback Method
dvisc	0.0007953	Pa×s	384.98	Joback Method
dvisc	0.0005675	Pa×s	420.05	Joback Method
dvisc	0.0004266	Pa×s	455.11	Joback Method
dvisc	0.0003340	Pa×s	490.18	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	354.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54134e+01
Coeff. B	-4.23073e+03
Coeff. C	-7.10180e+01
Temperature range (K), min.	350.72
Temperature range (K), max.	489.82

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C14090870&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume