2,3-Octanedione

Other names: 2,3-Octandione
Octane-2,3-dione
2,3-Octadione
Inchi: InChI=1S/C8H14O2/c1-3-4-5-6-8(10)7(2)9/h3-6H2,1-2H3
InchiKey: XCBBNTFYSLADTO-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCCCCC(=O)C(C)=O
Mol. weight [g/mol]: 142.20
CAS: 585-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-241.36	kJ/mol	Joback Method
hf	-433.61	kJ/mol	Joback Method
hfus	19.67	kJ/mol	Joback Method
hvap	46.89	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.725		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
rinpol	980.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	966.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	995.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	964.00		NIST Webbook

rinpol	983.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	967.00		NIST Webbook
rinpol	982.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	984.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	971.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	959.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	968.00		NIST Webbook
rinpol	981.00		NIST Webbook
rinpol	980.00		NIST Webbook
ripol	1322.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1335.00		NIST Webbook
ripol	1336.00		NIST Webbook
ripol	1342.00		NIST Webbook
ripol	1360.00		NIST Webbook
ripol	1325.00		NIST Webbook
ripol	1376.00		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	328.98	J/mol×K	644.98	Joback Method
cpg	319.22	J/mol×K	614.02	Joback Method
cpg	308.97	J/mol×K	583.06	Joback Method
cpg	298.23	J/mol×K	552.10	Joback Method
cpg	286.97	J/mol×K	521.14	Joback Method
cpg	338.27	J/mol×K	675.94	Joback Method
dvisc	0.0003340	Pa×s	490.18	Joback Method
dvisc	0.0004266	Pa×s	455.11	Joback Method
dvisc	0.0005675	Pa×s	420.05	Joback Method
dvisc	0.0007953	Pa×s	384.98	Joback Method
dvisc	0.0011925	Pa×s	349.91	Joback Method
dvisc	0.0019569	Pa×s	314.85	Joback Method
dvisc	0.0036359	Pa×s	279.78	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C585251&Units=SI
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
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