2,5-Octanedione

Other names: octane-2,5-dione
Inchi: InChI=1S/C8H14O2/c1-3-4-8(10)6-5-7(2)9/h3-6H2,1-2H3
InchiKey: SPDFSSLYVRCMDZ-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCCC(=O)CCC(C)=O
Mol. weight [g/mol]: 142.20
CAS: 3214-41-3

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	986.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
rinpol	983.00		NIST Webbook
rinpol	980.00		NIST Webbook
rinpol	985.00		NIST Webbook
rinpol	983.00		NIST Webbook
ripol	1319.00		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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	372.00 ± 1.00	K	1.60	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=C3214413&Units=SI

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

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