3,6-octanedione

Inchi: InChI=1S/C8H14O2/c1-3-7(9)5-6-8(10)4-2/h3-6H2,1-2H3
InchiKey: CVZGUJMLZZTPKH-UHFFFAOYSA-N
Formula: C8H14O2
SMILES: CCC(=O)CCC(=O)CC
Mol. weight [g/mol]: 142.20
CAS: 2955-65-9

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
ripol	1638.00		NIST Webbook
tb	484.40 ± 2.00	K	NIST Webbook
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

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.42922e+01
Coeff. B	-3.82516e+03
Coeff. C	-6.75200e+01
Temperature range (K), min.	340.66
Temperature range (K), max.	493.45

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2955659&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/38-405-0/3-6-octanedione.pdf
Generated by Cheméo on 2024-04-18 03:48:58.94629552 +0000 UTC m=+15701387.866872830.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.