4,5-Octanedione

Other names:	4,5-Octadione
	Bibutyryl
	n-Octane-4,5-dione
	octane-4,5-dione
Inchi:	InChI=1S/C8H14O2/c1-3-5-7(9)8(10)6-4-2/h3-6H2,1-2H3
InchiKey:	XYZAPOXYXNIBEU-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CCCC(=O)C(=O)CCC
Mol. weight [g/mol]:	142.20
CAS:	5455-24-3

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
tb	441.20	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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	333.20	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49754e+01
Coeff. B	-3.90888e+03
Coeff. C	-6.37900e+01
Temperature range (K), min.	329.92
Temperature range (K), max.	468.27

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C5455243&Units=SI

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