2,6-Heptanedione

Other names: 2,6-Heptadione
heptane-2,6-dione
Inchi: InChI=1S/C7H12O2/c1-6(8)4-3-5-7(2)9/h3-5H2,1-2H3
InchiKey: VAIFYHGFLAPCON-UHFFFAOYSA-N
Formula: C7H12O2
SMILES: CC(=O)CCCC(C)=O
Mol. weight [g/mol]: 128.17
CAS: 13505-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-249.78	kJ/mol	Joback Method
hf	-412.97	kJ/mol	Joback Method
hfus	17.08	kJ/mol	Joback Method
hvap	44.67	kJ/mol	Joback Method
log10ws	-1.31		Crippen Method
logp	1.335		Crippen Method
mcvol	112.630	ml/mol	McGowan Method
pc	3213.68	kPa	Joback Method
tb	467.30	K	Joback Method
tc	655.05	K	Joback Method
tf	304.95 ± 0.50	K	NIST Webbook
vc	0.440	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	233.34	J/mol×K	467.30	Joback Method
cpg	244.05	J/mol×K	498.59	Joback Method
cpg	254.28	J/mol×K	529.88	Joback Method
cpg	264.05	J/mol×K	561.18	Joback Method
cpg	273.38	J/mol×K	592.47	Joback Method
cpg	282.27	J/mol×K	623.76	Joback Method
cpg	290.73	J/mol×K	655.05	Joback Method

dvisc	0.0035564	Pa×s	268.51	Joback Method
dvisc	0.0019557	Pa×s	301.64	Joback Method
dvisc	0.0012106	Pa×s	334.77	Joback Method
dvisc	0.0008169	Pa×s	367.90	Joback Method
dvisc	0.0005883	Pa×s	401.04	Joback Method
dvisc	0.0004455	Pa×s	434.17	Joback Method
dvisc	0.0003508	Pa×s	467.30	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.34643e+01
Coeff. B	-6.82132e+03
Coeff. C	-7.88020e+01
Temperature range (K), min.	373.12
Temperature range (K), max.	454.57

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13505345&Units=SI

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

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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