Acetyl valeryl

Other names:	2,3-Heptanedione
	Valerylacetyl
	heptane-2,3-dione
Inchi:	InChI=1S/C7H12O2/c1-3-4-5-7(9)6(2)8/h3-5H2,1-2H3
InchiKey:	FJPGAMCQJNLTJC-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCCCC(=O)C(C)=O
Mol. weight [g/mol]:	128.17
CAS:	96-04-8

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
rinpol	816.00		NIST Webbook
rinpol	816.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1153.00		NIST Webbook
ripol	1138.00		NIST Webbook
ripol	1153.00		NIST Webbook
tb	467.30	K	Joback Method
tc	655.05	K	Joback Method
tf	268.51	K	Joback Method
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	1.30645e+01
Coeff. B	-3.24025e+03
Coeff. C	-5.71180e+01
Temperature range (K), min.	310.72
Temperature range (K), max.	475.05

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=C96048&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
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