2,4-Heptanedione

Other names:	Butanoylacetone
	Butyrylacetone
	heptane-2,4-dione
Inchi:	InChI=1S/C7H12O2/c1-3-4-7(9)5-6(2)8/h3-5H2,1-2H3
InchiKey:	ILPNRWUGFSPGAA-UHFFFAOYSA-N
Formula:	C7H12O2
SMILES:	CCCC(=O)CC(C)=O
Mol. weight [g/mol]:	128.17
CAS:	7307-02-0

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	982.81		NIST Webbook
rinpol	991.08		NIST Webbook
rinpol	977.42		NIST Webbook
rinpol	983.82		NIST Webbook
tb	447.20	K	NIST Webbook
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	282.27	J/mol×K	623.76	Joback Method

cpg	273.38	J/mol×K	592.47	Joback Method
cpg	264.05	J/mol×K	561.18	Joback Method
cpg	254.28	J/mol×K	529.88	Joback Method
cpg	244.05	J/mol×K	498.59	Joback Method
cpg	290.73	J/mol×K	655.05	Joback Method
dvisc	0.0003508	Pa×s	467.30	Joback Method
dvisc	0.0004455	Pa×s	434.17	Joback Method
dvisc	0.0005883	Pa×s	401.04	Joback Method
dvisc	0.0008169	Pa×s	367.90	Joback Method
dvisc	0.0012106	Pa×s	334.77	Joback Method
dvisc	0.0019557	Pa×s	301.64	Joback Method
dvisc	0.0035564	Pa×s	268.51	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	343.20	K	2.70	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=C7307020&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume