2,6-Heptanedione, 3-acetyl-

Other names: 3-acetylheptane-2,6-dione
Inchi: InChI=1S/C9H14O3/c1-6(10)4-5-9(7(2)11)8(3)12/h9H,4-5H2,1-3H3
InchiKey: RQZJIXZNJBCGQC-UHFFFAOYSA-N
Formula: C9H14O3
SMILES: CC(=O)CCC(C(C)=O)C(C)=O
Mol. weight [g/mol]: 170.21
CAS: 29214-57-1

Physical Properties

Property code	Value	Unit	Source
gf	-364.30	kJ/mol	Joback Method
hf	-572.11	kJ/mol	Joback Method
hfus	20.34	kJ/mol	Joback Method
hvap	55.48	kJ/mol	Joback Method
log10ws	-1.19		Crippen Method
logp	1.150		Crippen Method
mcvol	142.380	ml/mol	McGowan Method
pc	2814.34	kPa	Joback Method
tb	566.49	K	Joback Method
tc	762.62	K	Joback Method
tf	325.98	K	Joback Method
vc	0.551	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	337.30	J/mol×K	566.49	Joback Method
cpg	349.37	J/mol×K	599.18	Joback Method
cpg	360.81	J/mol×K	631.87	Joback Method
cpg	371.65	J/mol×K	664.55	Joback Method
cpg	381.90	J/mol×K	697.24	Joback Method
cpg	391.56	J/mol×K	729.93	Joback Method
cpg	400.67	J/mol×K	762.62	Joback Method
dvisc	0.0038903	Pa×s	325.98	Joback Method

dvisc	0.0020314	Pa×s	366.06	Joback Method
dvisc	0.0012059	Pa×s	406.15	Joback Method
dvisc	0.0007862	Pa×s	446.24	Joback Method
dvisc	0.0005500	Pa×s	486.32	Joback Method
dvisc	0.0004063	Pa×s	526.40	Joback Method
dvisc	0.0003133	Pa×s	566.49	Joback Method

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=C29214571&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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