2,4-Heptanedione, 3,5-dimethyl

Inchi: InChI=1S/C9H16O2/c1-5-6(2)9(11)7(3)8(4)10/h6-7H,5H2,1-4H3
InchiKey: XYXWCCLFDBKNCB-UHFFFAOYSA-N
Formula: C9H16O2
SMILES: CCC(C)C(=O)C(C)C(C)=O
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-237.82	kJ/mol	Joback Method
hf	-464.81	kJ/mol	Joback Method
hfus	15.22	kJ/mol	Joback Method
hvap	48.34	kJ/mol	Joback Method
log10ws	-1.67		Crippen Method
logp	1.827		Crippen Method
mcvol	140.810	ml/mol	McGowan Method
pc	2657.03	kPa	Joback Method
rinpol	1068.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	512.18	K	Joback Method
tc	703.77	K	Joback Method
tf	261.05	K	Joback Method
vc	0.539	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.58	J/mol×K	512.18	Joback Method
cpg	332.99	J/mol×K	544.11	Joback Method
cpg	345.76	J/mol×K	576.04	Joback Method
cpg	357.91	J/mol×K	607.98	Joback Method
cpg	369.47	J/mol×K	639.91	Joback Method
cpg	380.44	J/mol×K	671.84	Joback Method
cpg	390.83	J/mol×K	703.77	Joback Method
dvisc	0.0071523	Pa×s	261.05	Joback Method

dvisc	0.0028688	Pa×s	302.91	Joback Method
dvisc	0.0014364	Pa×s	344.76	Joback Method
dvisc	0.0008354	Pa×s	386.62	Joback Method
dvisc	0.0005402	Pa×s	428.47	Joback Method
dvisc	0.0003774	Pa×s	470.33	Joback Method
dvisc	0.0002796	Pa×s	512.18	Joback Method

Sources

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=R199567&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
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