2,6-Dimethyl-5-oxo-heptanoic acid

Inchi: InChI=1S/C9H16O3/c1-6(2)8(10)5-4-7(3)9(11)12/h6-7H,4-5H2,1-3H3,(H,11,12)
InchiKey: KFSWOOWOYKTCDK-UHFFFAOYSA-N
Formula: C9H16O3
SMILES: CC(C)C(=O)CCC(C)C(=O)O
Mol. weight [g/mol]: 172.22

Physical Properties

Property code	Value	Unit	Source
gf	-374.64	kJ/mol	Joback Method
hf	-617.04	kJ/mol	Joback Method
hfus	19.31	kJ/mol	Joback Method
hvap	65.02	kJ/mol	Joback Method
log10ws	-1.49		Crippen Method
logp	1.712		Crippen Method
mcvol	146.680	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
ripol	2515.00		NIST Webbook
tb	604.36	K	Joback Method
tc	786.29	K	Joback Method
tf	321.87	K	Joback Method
vc	0.558	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	373.45	J/mol×K	604.36	Joback Method
cpg	384.73	J/mol×K	634.68	Joback Method
cpg	395.46	J/mol×K	665.00	Joback Method
cpg	405.65	J/mol×K	695.32	Joback Method
cpg	415.32	J/mol×K	725.64	Joback Method
cpg	424.48	J/mol×K	755.97	Joback Method
cpg	433.14	J/mol×K	786.29	Joback Method
dvisc	0.0137516	Pa×s	321.87	Joback Method
dvisc	0.0035083	Pa×s	368.95	Joback Method

dvisc	0.0012193	Pa×s	416.03	Joback Method
dvisc	0.0005254	Pa×s	463.12	Joback Method
dvisc	0.0002644	Pa×s	510.20	Joback Method
dvisc	0.0001495	Pa×s	557.28	Joback Method
dvisc	0.0000923	Pa×s	604.36	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326100&Units=SI
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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