3,7-Dimethyl-6-oxo-octanoic acid

Inchi: InChI=1S/C10H18O3/c1-7(2)9(11)5-4-8(3)6-10(12)13/h7-8H,4-6H2,1-3H3,(H,12,13)
InchiKey: SCOSFCLSJUKLDZ-UHFFFAOYSA-N
Formula: C10H18O3
SMILES: CC(CCC(=O)C(C)C)CC(=O)O
Mol. weight [g/mol]: 186.25

Physical Properties

Property code	Value	Unit	Source
gf	-366.22	kJ/mol	Joback Method
hf	-637.68	kJ/mol	Joback Method
hfus	21.90	kJ/mol	Joback Method
hvap	67.25	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	2.103		Crippen Method
mcvol	160.770	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
ripol	2660.00		NIST Webbook
tb	627.24	K	Joback Method
tc	807.71	K	Joback Method
tf	333.14	K	Joback Method
vc	0.615	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.23	J/mol×K	627.24	Joback Method
cpg	434.21	J/mol×K	657.32	Joback Method
cpg	445.59	J/mol×K	687.40	Joback Method
cpg	456.41	J/mol×K	717.47	Joback Method
cpg	466.67	J/mol×K	747.55	Joback Method
cpg	476.38	J/mol×K	777.63	Joback Method
cpg	485.58	J/mol×K	807.71	Joback Method
dvisc	0.0112567	Pa×s	333.14	Joback Method
dvisc	0.0028810	Pa×s	382.16	Joback Method

dvisc	0.0010052	Pa×s	431.17	Joback Method
dvisc	0.0004348	Pa×s	480.19	Joback Method
dvisc	0.0002197	Pa×s	529.21	Joback Method
dvisc	0.0001246	Pa×s	578.22	Joback Method
dvisc	0.0000772	Pa×s	627.24	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=R326175&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume