4,6-Dioxoheptanoic acid

Other names:	Heptanoic acid, 4,6-dioxo- SA
Inchi:	InChI=1S/C7H10O4/c1-5(8)4-6(9)2-3-7(10)11/h2-4H2,1H3,(H,10,11)
InchiKey:	WYEPBHZLDUPIOD-UHFFFAOYSA-N
Formula:	C7H10O4
SMILES:	CC(=O)CC(=O)CCC(=O)O
Mol. weight [g/mol]:	158.15
CAS:	51568-18-4

Physical Properties

Property code	Value	Unit	Source
gf	-515.52	kJ/mol	Joback Method
hf	-677.78	kJ/mol	Joback Method
hfus	22.77	kJ/mol	Joback Method
hvap	68.09	kJ/mol	Joback Method
log10ws	-0.41		Crippen Method
logp	0.399		Crippen Method
mcvol	120.070	ml/mol	McGowan Method
pc	3862.67	kPa	Joback Method
rinpol	1350.40		NIST Webbook
rinpol	1350.40		NIST Webbook
tb	613.35	K	Joback Method
tc	799.87	K	Joback Method
tf	379.26	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.45	J/mol×K	613.35	Joback Method
cpg	299.76	J/mol×K	644.44	Joback Method
cpg	307.62	J/mol×K	675.52	Joback Method
cpg	315.07	J/mol×K	706.61	Joback Method
cpg	322.09	J/mol×K	737.70	Joback Method

cpg	328.72	J/mol×K	768.79	Joback Method
cpg	334.94	J/mol×K	799.87	Joback Method
dvisc	0.0039918	Pa×s	379.26	Joback Method
dvisc	0.0017181	Pa×s	418.28	Joback Method
dvisc	0.0008539	Pa×s	457.29	Joback Method
dvisc	0.0004737	Pa×s	496.31	Joback Method
dvisc	0.0002863	Pa×s	535.32	Joback Method
dvisc	0.0001853	Pa×s	574.34	Joback Method
dvisc	0.0001268	Pa×s	613.35	Joback Method

Sources

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=C51568184&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume