4-Ketopimelic

Other names:	«gamma»-Ketopimelic acid
	Heptanedioic acid, 4-oxo-
	4-Oxoheptanedioic acid
	4-Oxopimelic acid
Inchi:	InChI=1S/C7H10O5/c8-5(1-3-6(9)10)2-4-7(11)12/h1-4H2,(H,9,10)(H,11,12)
InchiKey:	UDDSEESQRGPVIL-UHFFFAOYSA-N
Formula:	C7H10O5
SMILES:	O=C(O)CCC(=O)CCC(=O)O
Mol. weight [g/mol]:	174.15
CAS:	502-50-1

Physical Properties

Property code	Value	Unit	Source
gf	-652.34	kJ/mol	Joback Method
hf	-830.01	kJ/mol	Joback Method
hfus	26.86	kJ/mol	Joback Method
hvap	84.77	kJ/mol	Joback Method
log10ws	-0.23		Crippen Method
logp	0.285		Crippen Method
mcvol	125.940	ml/mol	McGowan Method
pc	4345.39	kPa	Joback Method
tb	705.53	K	Joback Method
tc	886.49	K	Joback Method
tf	440.08	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	332.39	J/mol×K	705.53	Joback Method
cpg	363.51	J/mol×K	856.33	Joback Method
cpg	358.04	J/mol×K	826.17	Joback Method
cpg	352.21	J/mol×K	796.01	Joback Method
cpg	345.99	J/mol×K	765.85	Joback Method

cpg	339.39	J/mol×K	735.69	Joback Method
cpg	368.63	J/mol×K	886.49	Joback Method
dvisc	0.0000224	Pa×s	705.53	Joback Method
dvisc	0.0000365	Pa×s	661.29	Joback Method
dvisc	0.0000638	Pa×s	617.05	Joback Method
dvisc	0.0001215	Pa×s	572.81	Joback Method
dvisc	0.0002577	Pa×s	528.56	Joback Method
dvisc	0.0006272	Pa×s	484.32	Joback Method
dvisc	0.0018257	Pa×s	440.08	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C502501&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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