

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/molxK	705.53	Joback Method
cpg	363.51	J/molxK	856.33	Joback Method
cpg	358.04	J/molxK	826.17	Joback Method
cpg	352.21	J/molxK	796.01	Joback Method
cpg	345.99	J/molxK	765.85	Joback Method

cpg	339.39	J/molxK	735.69	Joback Method
cpg	368.63	J/molxK	886.49	Joback Method
dvisc	0.0000224	Paxs	705.53	Joback Method
dvisc	0.0000365	Paxs	661.29	Joback Method
dvisc	0.0000638	Paxs	617.05	Joback Method
dvisc	0.0001215	Paxs	572.81	Joback Method
dvisc	0.0002577	Paxs	528.56	Joback Method
dvisc	0.0006272	Paxs	484.32	Joback Method
dvisc	0.0018257	Paxs	440.08	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C502501&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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