

2-Oxoadipic acid

Other names:	Hexanedioic acid, 2-oxo- «alpha»-Ketoadipic acid 2-Oxohexanedioic acid
Inchi:	InChI=1S/C6H8O5/c7-4(6(10)11)2-1-3-5(8)9/h1-3H2,(H,8,9)(H,10,11)
InchiKey:	FGSBNBBHOZHUBO-UHFFFAOYSA-N
Formula:	C6H8O5
SMILES:	O=C(O)CCCC(=O)C(=O)O
Mol. weight [g/mol]:	160.12
CAS:	3184-35-8

Physical Properties

Property code	Value	Unit	Source
gf	-660.76	kJ/mol	Joback Method
hf	-809.37	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	82.55	kJ/mol	Joback Method
log10ws	0.19		Crippen Method
logp	-0.105		Crippen Method
mcvol	111.850	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
tb	682.65	K	Joback Method
tc	864.07	K	Joback Method
tf	428.81	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	284.43	J/mol×K	682.65	Joback Method
cpg	290.65	J/mol×K	712.89	Joback Method
cpg	296.52	J/mol×K	743.12	Joback Method
cpg	302.05	J/mol×K	773.36	Joback Method
cpg	307.23	J/mol×K	803.60	Joback Method
cpg	312.09	J/mol×K	833.83	Joback Method

cpg	316.62	J/mol×K	864.07	Joback Method
dvisc	0.0022363	Pa×s	428.81	Joback Method
dvisc	0.0007762	Pa×s	471.12	Joback Method
dvisc	0.0003207	Pa×s	513.42	Joback Method
dvisc	0.0001516	Pa×s	555.73	Joback Method
dvisc	0.0000797	Pa×s	598.04	Joback Method
dvisc	0.0000456	Pa×s	640.34	Joback Method
dvisc	0.0000280	Pa×s	682.65	Joback Method
hsubt	127.00	kJ/mol	291.00	NIST Webbook

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3184358&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
hsubt:	Enthalpy of sublimation at a given temperature
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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