alpha-KETOADIPIC 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]: 160.13

Physical Properties

Property code	Value	Unit	Source
gf	-660.76	kJ/mol	Joback Method
hf	-926.76	kJ/mol	Cheméo Relay (1.0)
hfus	24.27	kJ/mol	Joback Method
hvap	103.77	kJ/mol	Cheméo Relay (1.0)
ie	10.05	eV	Cheméo Relay (1.0)
log10ws	-0.06		Cheméo Relay (1.0)
logp	-0.105		Crippen Method
mcvol	111.850	ml/mol	McGowan Method
pc	4952.36	kPa	Joback Method
tb	531.69	K	Cheméo Relay (1.0)
tc	795.05	K	Cheméo Relay (1.0)
tf	397.95	K	Cheméo Relay (1.0)
vc	0.413	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	312.09	J/mol×K	833.83	Joback Method
cpg	316.62	J/mol×K	864.07	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	284.43	J/mol×K	682.65	Joback Method
dvisc	0.0003207	Pa×s	513.42	Joback Method
dvisc	0.0007762	Pa×s	471.12	Joback Method
dvisc	0.0022363	Pa×s	428.81	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

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3184358&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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
ie: Ionization energy
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