2-Oxopentanedioic acid

Other names:	2-Ketoglutaric acid 2-Oxoglutaric acid «alpha»-Ketoglutaric acid Pentanedioic acid, 2-oxo- Glutaric acid, 2-oxo- Glutaric acid, «alpha»-keto- 2-Oxo-1,5-pentanedioic acid NSC 17391 «alpha»-Oxoglutaric acid
Inchi:	InChI=1S/C5H6O5/c6-3(5(9)10)1-2-4(7)8/h1-2H2,(H,7,8)(H,9,10)
InchiKey:	KPGXRSRHYNQIFN-UHFFFAOYSA-N
Formula:	C5H6O5
SMILES:	O=C(O)CCC(=O)C(=O)O
Mol. weight [g/mol]:	146.10
CAS:	328-50-7

Physical Properties

Property code	Value	Unit	Source
chs	-1801.11	kJ/mol	NIST Webbook
chs	-1798.90 ± 0.84	kJ/mol	NIST Webbook
gf	-669.18	kJ/mol	Joback Method
hf	-788.73	kJ/mol	Joback Method
hfs	-1026.20 ± 0.88	kJ/mol	NIST Webbook
hfs	-1027.89	kJ/mol	NIST Webbook
hfus	21.68	kJ/mol	Joback Method
hvap	80.32	kJ/mol	Joback Method
log10ws	0.61		Crippen Method
logp	-0.495		Crippen Method
mcvol	97.760	ml/mol	McGowan Method
pc	5695.98	kPa	Joback Method
tb	659.77	K	Joback Method
tc	842.08	K	Joback Method
tf	390.90 ± 1.00	K	NIST Webbook
tf	388.45 ± 1.50	K	NIST Webbook
vc	0.371	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.97	J/mol×K	659.77	Joback Method
cpg	243.35	J/mol×K	690.16	Joback Method
cpg	248.42	J/mol×K	720.54	Joback Method
cpg	253.19	J/mol×K	750.93	Joback Method
cpg	257.66	J/mol×K	781.31	Joback Method
cpg	261.84	J/mol×K	811.70	Joback Method
cpg	265.74	J/mol×K	842.08	Joback Method
dvisc	0.0009585	Pa×s	457.91	Joback Method
dvisc	0.0027311	Pa×s	417.54	Joback Method
dvisc	0.0003986	Pa×s	498.28	Joback Method
dvisc	0.0001891	Pa×s	538.65	Joback Method
dvisc	0.0000995	Pa×s	579.03	Joback Method
dvisc	0.0000569	Pa×s	619.40	Joback Method
dvisc	0.0000349	Pa×s	659.77	Joback Method
hfust	28.59	kJ/mol	388.70	NIST Webbook
hsubt	100.00	kJ/mol	277.00	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=C328507&Units=SI

Legend

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions

hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
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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