

Oxalacetic acid

Other names:	Oxaloacetic acid Butanedioic acid, oxo- Ketosuccinic acid Oxosuccinic acid OAA 2-Ketosuccinic acid 2-Oxosuccinic acid Butanedioic acid, 2-oxo- NSC 77688
Inchi:	InChI=1S/C4H4O5/c5-2(4(8)9)1-3(6)7/h1H2,(H,6,7)(H,8,9)
InchiKey:	KHPXUQMNIQBQEV-UHFFFAOYSA-N
Formula:	C4H4O5
SMILES:	O=C(O)CC(=O)C(=O)O
Mol. weight [g/mol]:	132.07
CAS:	328-42-7

Physical Properties

Property code	Value	Unit	Source
chs	-1205.58	kJ/mol	NIST Webbook
gf	-677.60	kJ/mol	Joback Method
hf	-768.09	kJ/mol	Joback Method
hfs	-943.21	kJ/mol	NIST Webbook
hfus	19.09	kJ/mol	Joback Method
hvap	78.09	kJ/mol	Joback Method
log10ws	1.02		Crippen Method
logp	-0.885		Crippen Method
mcvol	83.670	ml/mol	McGowan Method
pc	6620.58	kPa	Joback Method
tb	636.89	K	Joback Method
tc	820.48	K	Joback Method
tf	406.27	K	Joback Method
vc	0.316	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.10	J/molxK	636.89	Joback Method
cpg	212.81	J/molxK	789.88	Joback Method
cpg	209.38	J/molxK	759.28	Joback Method
cpg	205.70	J/molxK	728.68	Joback Method
cpg	201.76	J/molxK	698.09	Joback Method
cpg	197.56	J/molxK	667.49	Joback Method
cpg	216.01	J/molxK	820.48	Joback Method
dvisc	0.0000435	Paxs	636.89	Joback Method
dvisc	0.0000710	Paxs	598.45	Joback Method
dvisc	0.0001241	Paxs	560.02	Joback Method
dvisc	0.0002353	Paxs	521.58	Joback Method
dvisc	0.0004942	Paxs	483.14	Joback Method
dvisc	0.0011800	Paxs	444.71	Joback Method
dvisc	0.0033217	Paxs	406.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C328427&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

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
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

Latest version available from:

<https://www.cheméo.com/cid/39-860-4/Oxalacetic-acid.pdf>

Generated by Cheméo on 2024-04-27 08:08:53.277880036 +0000 UTC m=+16494582.198457348.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.