

2,3-Dimethylsuccinic acid

Other names:	«alpha», «beta»-Dimethylsuccinic acid Butanedioic acid, 2,3-dimethyl- Succinic acid, 2,3-dimethyl- 2,3-Butanedicarboxylic acid
Inchi:	InChI=1S/C6H10O4/c1-3(5(7)8)4(2)6(9)10/h3-4H,1-2H3,(H,7,8)(H,9,10)
InchiKey:	KLZYRCVPDWTZLH-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(C(=O)O)C(C)C(=O)O
Mol. weight [g/mol]:	146.14
CAS:	13545-04-5

Physical Properties

Property code	Value	Unit	Source
gf	-536.72	kJ/mol	Joback Method
hf	-707.35	kJ/mol	Joback Method
hfus	15.62	kJ/mol	Joback Method
hvap	75.02	kJ/mol	Joback Method
log10ws	-0.05		Crippen Method
logp	0.428		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4640.32	kPa	Joback Method
tb	627.90	K	Joback Method
tc	807.19	K	Joback Method
tf	413.00 ± 3.00	K	NIST Webbook
vc	0.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.61	J/mol×K	627.90	Joback Method
cpg	285.95	J/mol×K	657.78	Joback Method
cpg	292.90	J/mol×K	687.66	Joback Method
cpg	299.49	J/mol×K	717.55	Joback Method
cpg	305.72	J/mol×K	747.43	Joback Method

cpg	311.60	J/molxK	777.31	Joback Method
cpg	317.14	J/molxK	807.19	Joback Method
dvisc	0.0165669	Paxs	348.88	Joback Method
dvisc	0.0031943	Paxs	395.38	Joback Method
dvisc	0.0008709	Paxs	441.89	Joback Method
dvisc	0.0003041	Paxs	488.39	Joback Method
dvisc	0.0001275	Paxs	534.89	Joback Method
dvisc	0.0000614	Paxs	581.40	Joback Method
dvisc	0.0000330	Paxs	627.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C13545045&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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