2,2-Dimethylbutanedioic acid

Other names:	1,4-butanedioic acid, 2,2-dimethyl- 2,2-Dimethylsuccinic acid 2,2-dimethyl-1,4-butanedioic acid Butanedioic acid, 2,2-dimethyl- Succinic acid, 2,2-dimethyl-
Inchi:	InChI=1S/C6H10O4/c1-6(2,5(9)10)3-4(7)8/h3H2,1-2H3,(H,7,8)(H,9,10)
InchiKey:	GOHPTLYPQCTZSE-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(C)(CC(=O)O)C(=O)O
Mol. weight [g/mol]:	146.14
CAS:	597-43-3

Physical Properties

Property code	Value	Unit	Source
chs	-2802.40 ± 1.40	kJ/mol	NIST Webbook
gf	-529.00	kJ/mol	Joback Method
hf	-705.54	kJ/mol	Joback Method
hfus	38.11	kJ/mol	Solid Liquid Equilibria for Six Binary Mixtures of Pentanedioic Acid, Octanedioic Acid, 3-Methylheptanedioic Acid, 2,2-Dimethylbutanedioic Acid, and 2,3-Dimethylbutanedioic Acid
hvap	74.50	kJ/mol	Joback Method
log10ws	-0.29		Crippen Method
logp	0.572		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4659.34	kPa	Joback Method
tb	625.55	K	Joback Method
tc	807.18	K	Joback Method
tf	410.15 ± 2.00	K	NIST Webbook
tf	414.15 ± 1.50	K	NIST Webbook
tf	412.15 ± 1.50	K	NIST Webbook
tf	408.00 ± 5.00	K	NIST Webbook
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	281.34	J/mol×K	625.55	Joback Method
cpg	288.56	J/mol×K	655.82	Joback Method
cpg	295.34	J/mol×K	686.09	Joback Method
cpg	301.72	J/mol×K	716.36	Joback Method
cpg	307.71	J/mol×K	746.63	Joback Method
cpg	313.33	J/mol×K	776.90	Joback Method
cpg	318.62	J/mol×K	807.18	Joback Method
dvisc	0.0059533	Pa×s	381.30	Joback Method
dvisc	0.0016603	Pa×s	422.01	Joback Method
dvisc	0.0005797	Pa×s	462.72	Joback Method
dvisc	0.0002399	Pa×s	503.42	Joback Method
dvisc	0.0001133	Pa×s	544.13	Joback Method
dvisc	0.0000594	Pa×s	584.84	Joback Method
dvisc	0.0000339	Pa×s	625.55	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.93402e+01
Coeff. B	-7.00404e+03
Coeff. C	-1.08784e+02
Temperature range (K), min.	476.40
Temperature range (K), max.	608.05

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid Liquid Equilibria for Six Binary Mixtures of Pentanedioic Acid, Octanedioic Acid, 3-Methylheptanedioic Acid, 2,2-Dimethylbutanedioic Acid, and 2,3-Dimethylbutanedioic Acid:	https://www.doi.org/10.1021/je400686f

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=C597433&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume