

2,2-Dimethylglutaric acid

Other names:	Pentanedioic acid, 2,2-dimethyl- «alpha», «alpha»-Dimethylglutaric acid Â«alphaÂ», Â«alphaÂ»-Dimethylglutaric acid
Inchi:	InChI=1S/C7H12O4/c1-7(2,6(10)11)4-3-5(8)9/h3-4H2,1-2H3,(H,8,9)(H,10,11)
InchiKey:	BTUDGPVTCYNYLK-UHFFFAOYSA-N
Formula:	C7H12O4
SMILES:	CC(C)(CCC(=O)O)C(=O)O
Mol. weight [g/mol]:	160.17
CAS:	681-57-2

Physical Properties

Property code	Value	Unit	Source
gf	-520.58	kJ/mol	Joback Method
hf	-726.18	kJ/mol	Joback Method
hfus	17.85	kJ/mol	Joback Method
hvap	76.73	kJ/mol	Joback Method
log10ws	-0.71		Crippen Method
logp	0.962		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	648.43	K	Joback Method
tc	828.81	K	Joback Method
tf	413.00 ± 2.00	K	NIST Webbook
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.90	J/molxK	648.43	Joback Method
cpg	363.51	J/molxK	798.75	Joback Method
cpg	357.22	J/molxK	768.69	Joback Method
cpg	350.53	J/molxK	738.62	Joback Method
cpg	343.44	J/molxK	708.56	Joback Method
cpg	335.90	J/molxK	678.49	Joback Method

cpg	369.43	J/mol×K	828.81	Joback Method
dvisc	0.0000265	Paxs	648.43	Joback Method
dvisc	0.0000463	Paxs	605.79	Joback Method
dvisc	0.0000880	Paxs	563.14	Joback Method
dvisc	0.0001859	Paxs	520.50	Joback Method
dvisc	0.0004488	Paxs	477.86	Joback Method
dvisc	0.0012880	Paxs	435.21	Joback Method
dvisc	0.0046479	Paxs	392.57	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.73235e+01
Coeff. B	-6.26489e+03
Coeff. C	-1.08853e+02
Temperature range (K), min.	476.60
Temperature range (K), max.	630.41

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=C681572&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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