3,3-DIMETHYLGLUTARIC ACID

Other names: 3,3-Dimethylpentanedioic acid
Glutaric acid, 3,3-dimethyl-
Pentanedioic acid, 3,3-dimethyl-
«beta»,«beta»-Dimethylglutaric acid
Inchi: InChI=1S/C7H12O4/c1-7(2,3-5(8)9)4-6(10)11/h3-4H2,1-2H3,(H,8,9)(H,10,11)
InchiKey: DUHQIGLHYXLKAE-UHFFFAOYSA-N
Formula: C7H12O4
SMILES: CC(C)(CC(=O)O)CC(=O)O
Mol. weight [g/mol]: 160.17
CAS: 4839-46-7

Physical Properties

Property code	Value	Unit	Source
af	0.8066		Cheméo Relay (1.0)
gf	-520.58	kJ/mol	Joback Method
hf	-878.49	kJ/mol	Cheméo Relay (1.0)
hfus	17.85	kJ/mol	Joback Method
hvap	103.31	kJ/mol	Cheméo Relay (1.0)
ie	9.83	eV	Cheméo Relay (1.0)
log10ws	-0.46		Cheméo Relay (1.0)
logp	0.962		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	497.24	K	Cheméo Relay (1.0)
tc	732.69	K	Cheméo Relay (1.0)
tf	383.76	K	Cheméo Relay (1.0)
vc	0.426	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	327.90	J/mol×K	648.43	Joback Method
cpg	369.43	J/mol×K	828.81	Joback Method
cpg	363.51	J/mol×K	798.75	Joback Method

cpg	357.22	J/mol×K	768.69	Joback Method
cpg	350.53	J/mol×K	738.62	Joback Method
cpg	343.44	J/mol×K	708.56	Joback Method
cpg	335.90	J/mol×K	678.49	Joback Method
dvisc	0.0001859	Pa×s	520.50	Joback Method
dvisc	0.0000265	Pa×s	648.43	Joback Method
dvisc	0.0000463	Pa×s	605.79	Joback Method
dvisc	0.0000880	Pa×s	563.14	Joback Method
dvisc	0.0046479	Pa×s	392.57	Joback Method
dvisc	0.0004488	Pa×s	477.86	Joback Method
dvisc	0.0012880	Pa×s	435.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	362.70	K	0.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.77303e+01
Coeff. B	-6.45093e+03
Coeff. C	-1.09965e+02
Temperature range (K), min.	479.80
Temperature range (K), max.	629.41

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4839467&Units=SI

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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