

2-METHYLGLOUTARIC ACID

Inchi:	InChI=1S/C6H10O4/c1-4(6(9)10)2-3-5(7)8/h4H,2-3H2,1H3,(H,7,8)(H,9,10)
InchiKey:	AQYCMVICBNBXNA-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	CC(CCC(=O)O)C(=O)O
Mol. weight [g/mol]:	146.14
CAS:	18069-17-5

Physical Properties

Property code	Value	Unit	Source
af	0.7921		Cheméo Relay (1.0)
hf	-846.77	kJ/mol	Cheméo Relay (1.0)
hfus	19.15	kJ/mol	Joback Method
hvap	101.91	kJ/mol	Cheméo Relay (1.0)
ie	10.26	eV	Cheméo Relay (1.0)
log10ws	-0.05		Cheméo Relay (1.0)
logp	0.572		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	4590.15	kPa	Joback Method
tb	510.85	K	Cheméo Relay (1.0)
tc	732.99	K	Cheméo Relay (1.0)
tf	349.69	K	Cheméo Relay (1.0)
vc	0.392	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	278.07	J/mol×K	628.34	Joback Method
cpg	285.25	J/mol×K	657.76	Joback Method
cpg	292.08	J/mol×K	687.17	Joback Method
cpg	298.55	J/mol×K	716.59	Joback Method
cpg	304.69	J/mol×K	746.00	Joback Method
cpg	310.49	J/mol×K	775.42	Joback Method
cpg	315.96	J/mol×K	804.84	Joback Method
dvisc	0.0095884	Pa×s	363.88	Joback Method

dvisc	0.0022752	Pa×s	407.96	Joback Method
dvisc	0.0007147	Pa×s	452.03	Joback Method
dvisc	0.0002758	Pa×s	496.11	Joback Method
dvisc	0.0001243	Pa×s	540.19	Joback Method
dvisc	0.0000632	Pa×s	584.26	Joback Method
dvisc	0.0000353	Pa×s	628.34	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	487.70	K	2.90	NIST Webbook
tbrp	479.70	K	1.60	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.98753e+01
Coeff. B	-7.24164e+03
Coeff. C	-1.09896e+02
Temperature range (K), min.	479.60
Temperature range (K), max.	607.13

Sources

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=C18069175&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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