Methyl hydrogen glutarate

Other names:	Glutaric acid, monomethyl ester
	Methyl hydrogen glutarate
	Monomethyl glutarate
	Methyl glutarate,mono
	Monomethyl ester of glutaric acid
Inchi:	InChI=1S/C6H10O4/c1-10-6(9)4-2-3-5(7)8/h2-4H2,1H3,(H,7,8)
InchiKey:	IBMRTYCHDPMBFN-UHFFFAOYSA-N
Formula:	C6H10O4
SMILES:	COC(=O)CCCC(=O)O
Mol. weight [g/mol]:	146.14

Physical Properties

Property code	Value	Unit	Source
af	0.7327		Cheméo Relay (1.0)
gf	-500.02	kJ/mol	Joback Method
hf	-806.64	kJ/mol	Cheméo Relay (1.0)
hfus	19.77	kJ/mol	Joback Method
hvap	83.86	kJ/mol	Cheméo Relay (1.0)
ie	10.15	eV	Cheméo Relay (1.0)
log10ws	-0.11		Cheméo Relay (1.0)
logp	0.414		Crippen Method
mcvol	110.280	ml/mol	McGowan Method
pc	3940.66	kPa	Joback Method
tb	522.68	K	Cheméo Relay (1.0)
tc	699.53	K	Cheméo Relay (1.0)
tf	319.67	K	Cheméo Relay (1.0)
vc	0.408	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.90	J/mol×K	559.02	Joback Method
cpg	266.10	J/mol×K	588.95	Joback Method
cpg	273.95	J/mol×K	618.88	Joback Method

cpg	281.47	J/mol×K	648.80	Joback Method
cpg	288.64	J/mol×K	678.73	Joback Method
cpg	295.48	J/mol×K	708.66	Joback Method
cpg	301.97	J/mol×K	738.59	Joback Method
dvisc	0.0052745	Pa×s	340.29	Joback Method
dvisc	0.0021175	Pa×s	376.75	Joback Method
dvisc	0.0009987	Pa×s	413.20	Joback Method
dvisc	0.0005320	Pa×s	449.65	Joback Method
dvisc	0.0003115	Pa×s	486.11	Joback Method
dvisc	0.0001965	Pa×s	522.56	Joback Method
dvisc	0.0001317	Pa×s	559.02	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	423.70	K	1.30	NIST Webbook
tbrp	434.50 ± 3.50	K	3.10	NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1501275&Units=SI

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

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume