DIETHYLMALONIC ACID

Other names: Malonic acid, diethyl-
Diethylmalonic acid
3,3-Pentanedicarboxylic acid
Inchi: InChI=1S/C7H12O4/c1-3-7(4-2,5(8)9)6(10)11/h3-4H2,1-2H3,(H,8,9)(H,10,11)
InchiKey: LTMRRSWNXVJMBA-UHFFFAOYSA-N
Formula: C7H12O4
SMILES: CCC(CC)(C(=O)O)C(=O)O
Mol. weight [g/mol]: 160.17

Physical Properties

Property code	Value	Unit	Source
af	0.7641		Cheméo Relay (1.0)
gf	-520.58	kJ/mol	Joback Method
hf	-858.63	kJ/mol	Cheméo Relay (1.0)
hfus	17.85	kJ/mol	Joback Method
hvap	72.07	kJ/mol	Cheméo Relay (1.0)
ie	10.40	eV	NIST Webbook
logp	0.962		Crippen Method
mcvol	124.370	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	500.24	K	Cheméo Relay (1.0)
tc	735.86	K	Cheméo Relay (1.0)
tf	405.87	K	Cheméo Relay (1.0)
vc	0.423	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	335.90	J/mol×K	678.49	Joback Method
cpg	343.44	J/mol×K	708.56	Joback Method
cpg	350.53	J/mol×K	738.62	Joback Method
cpg	357.22	J/mol×K	768.69	Joback Method
cpg	363.51	J/mol×K	798.75	Joback Method

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

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C510203&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

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
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from: