[2H2]malonic [2H2]acid

Other names: Malonic acid-d4
Inchi: InChI=1S/C3H4O4/c4-2(5)1-3(6)7/h1H2,(H,4,5)(H,6,7)/i1D2/hD2
InchiKey: OFOBLEOULBTSOW-BGOGGDMHSA-N
Formula: C3D4O4
SMILES: O=C(O)CC(=O)O
Mol. weight [g/mol]: 108.09
CAS: 813-56-9

Physical Properties

Property code	Value	Unit	Source
gf	-557.10	kJ/mol	Joback Method
hf	-634.87	kJ/mol	Joback Method
hfus	14.90	kJ/mol	Joback Method
hvap	69.12	kJ/mol	Joback Method
log10ws	0.72		Crippen Method
logp	-0.454		Crippen Method
mcvol	68.010	ml/mol	McGowan Method
pc	6990.97	kPa	Joback Method
ss	157.14	J/mol×K	NIST Webbook
tb	560.14	K	Joback Method
tc	737.52	K	Joback Method
tf	345.07	K	Joback Method
vc	0.254	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	147.44	J/mol×K	560.14	Joback Method
cpg	151.57	J/mol×K	589.70	Joback Method
cpg	155.48	J/mol×K	619.27	Joback Method
cpg	159.20	J/mol×K	648.83	Joback Method
cpg	162.72	J/mol×K	678.39	Joback Method
cpg	166.05	J/mol×K	707.95	Joback Method
cpg	169.19	J/mol×K	737.52	Joback Method

cps	139.93	J/mol×K	298.15	NIST Webbook
dvisc	0.0115826	Pa×s	345.07	Joback Method
dvisc	0.0033725	Pa×s	380.92	Joback Method
dvisc	0.0012142	Pa×s	416.76	Joback Method
dvisc	0.0005139	Pa×s	452.61	Joback Method
dvisc	0.0002468	Pa×s	488.45	Joback Method
dvisc	0.0001310	Pa×s	524.30	Joback Method
dvisc	0.0000754	Pa×s	560.14	Joback Method

Sources

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=C813569&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg: Ideal gas heat capacity
cps: Solid phase 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
ss: Solid phase molar entropy at standard conditions
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume