Dimethylmalonic acid, ethyl heptyl ester

Inchi: InChI=1S/C14H26O4/c1-5-7-8-9-10-11-18-13(16)14(3,4)12(15)17-6-2/h5-11H2,1-4H3
InchiKey: MXPXVDMNLAXXEA-UHFFFAOYSA-N
Formula: C14H26O4
SMILES: CCCCCCCOC(=O)C(C)(C)C(=O)OCC
Mol. weight [g/mol]: 258.35

Physical Properties

Property code	Value	Unit	Source
gf	-398.00	kJ/mol	Joback Method
hf	-830.64	kJ/mol	Joback Method
hfus	30.18	kJ/mol	Joback Method
hvap	63.77	kJ/mol	Joback Method
log10ws	-3.17		Crippen Method
logp	3.089		Crippen Method
mcvol	223.000	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	1568.00		NIST Webbook
tb	669.07	K	Joback Method
tc	851.99	K	Joback Method
tf	394.28	K	Joback Method
vc	0.857	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	624.77	J/mol×K	669.07	Joback Method
cpg	640.85	J/mol×K	699.56	Joback Method
cpg	656.11	J/mol×K	730.04	Joback Method
cpg	670.56	J/mol×K	760.53	Joback Method
cpg	684.23	J/mol×K	791.02	Joback Method
cpg	697.13	J/mol×K	821.51	Joback Method
cpg	709.28	J/mol×K	851.99	Joback Method
dvisc	0.0015451	Pa×s	394.28	Joback Method
dvisc	0.0007767	Pa×s	440.08	Joback Method

dvisc	0.0004445	Pa×s	485.88	Joback Method
dvisc	0.0002800	Pa×s	531.67	Joback Method
dvisc	0.0001899	Pa×s	577.47	Joback Method
dvisc	0.0001363	Pa×s	623.27	Joback Method
dvisc	0.0001024	Pa×s	669.07	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U361898&Units=SI

Legend

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume