Malonic acid, 2,4-dimethylpent-3-yl ethyl ester

Inchi: InChI=1S/C12H22O4/c1-6-15-10(13)7-11(14)16-12(8(2)3)9(4)5/h8-9,12H,6-7H2,1-5H3
InchiKey: ANRPBMPCJBBSHU-UHFFFAOYSA-N
Formula: C12H22O4
SMILES: CCOC(=O)CC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]: 230.30

Physical Properties

Property code	Value	Unit	Source
gf	-425.00	kJ/mol	Joback Method
hf	-796.45	kJ/mol	Joback Method
hfus	21.84	kJ/mol	Joback Method
hvap	59.45	kJ/mol	Joback Method
log10ws	-2.20		Crippen Method
logp	2.163		Crippen Method
mcvol	194.820	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1398.00		NIST Webbook
tb	625.22	K	Joback Method
tc	811.54	K	Joback Method
tf	324.32	K	Joback Method
vc	0.738	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	517.23	J/mol×K	625.22	Joback Method
cpg	587.06	J/mol×K	780.49	Joback Method
cpg	574.54	J/mol×K	749.44	Joback Method
cpg	561.29	J/mol×K	718.38	Joback Method
cpg	547.33	J/mol×K	687.33	Joback Method
cpg	532.64	J/mol×K	656.27	Joback Method
cpg	598.87	J/mol×K	811.54	Joback Method
dvisc	0.0001230	Pa×s	625.22	Joback Method
dvisc	0.0001693	Pa×s	575.07	Joback Method

dvisc	0.0002477	Pa×s	524.92	Joback Method
dvisc	0.0003927	Pa×s	474.77	Joback Method
dvisc	0.0006943	Pa×s	424.62	Joback Method
dvisc	0.0014297	Pa×s	374.47	Joback Method
dvisc	0.0036813	Pa×s	324.32	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=U349008&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