Malonic acid, di(2,4-dimethylpent-3-yl) ester

Inchi: InChI=1S/C17H32O4/c1-10(2)16(11(3)4)20-14(18)9-15(19)21-17(12(5)6)13(7)8/h10-13,1
InchiKey: UCMHFRJIUYHQPK-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CC(C)C(OC(=O)CC(=O)OC(C(C)C)C(C)C)C(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-390.22	kJ/mol	Joback Method
hf	-915.49	kJ/mol	Joback Method
hfus	24.22	kJ/mol	Joback Method
hvap	69.42	kJ/mol	Joback Method
log10ws	-3.92		Crippen Method
logp	3.824		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1361.64	kPa	Joback Method
rinpol	1742.00		NIST Webbook
rinpol	1742.00		NIST Webbook
tb	738.30	K	Joback Method
tc	927.03	K	Joback Method
tf	335.67	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	793.93	J/mol×K	738.30	Joback Method
cpg	812.13	J/mol×K	769.75	Joback Method
cpg	829.29	J/mol×K	801.21	Joback Method
cpg	845.44	J/mol×K	832.66	Joback Method
cpg	860.57	J/mol×K	864.12	Joback Method
cpg	874.71	J/mol×K	895.57	Joback Method
cpg	887.87	J/mol×K	927.03	Joback Method
dvisc	0.0053329	Pa×s	335.67	Joback Method

dvisc	0.0012803	Pa×s	402.77	Joback Method
dvisc	0.0004620	Pa×s	469.88	Joback Method
dvisc	0.0002151	Pa×s	536.99	Joback Method
dvisc	0.0001187	Pa×s	604.09	Joback Method
dvisc	0.0000737	Pa×s	671.19	Joback Method
dvisc	0.0000500	Pa×s	738.30	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=U349025&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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