Dimethylmalonic acid, di(2-methylpent-3-yl) ester

Inchi: InChI=1S/C17H32O4/c1-9-13(11(3)4)20-15(18)17(7,8)16(19)21-14(10-2)12(5)6/h11-14H
InchiKey: RXSGWLRXFBEPEO-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCC(OC(=O)C(C)(C)C(=O)OC(CC)C(C)C)C(C)C
Mol. weight [g/mol]: 300.43

Physical Properties

Property code	Value	Unit	Source
gf	-382.50	kJ/mol	Joback Method
hf	-913.68	kJ/mol	Joback Method
hfus	23.85	kJ/mol	Joback Method
hvap	68.90	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.968		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	1740.00		NIST Webbook
rinpol	1740.00		NIST Webbook
tb	735.95	K	Joback Method
tc	926.53	K	Joback Method
tf	368.09	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.79	J/mol×K	735.95	Joback Method
cpg	875.06	J/mol×K	894.77	Joback Method
cpg	861.00	J/mol×K	863.00	Joback Method
cpg	845.97	J/mol×K	831.24	Joback Method
cpg	829.94	J/mol×K	799.48	Joback Method
cpg	812.89	J/mol×K	767.71	Joback Method
cpg	888.18	J/mol×K	926.53	Joback Method
dvisc	0.0000485	Pa×s	735.95	Joback Method

dvisc	0.0000706	Pa×s	674.64	Joback Method
dvisc	0.0001108	Pa×s	613.33	Joback Method
dvisc	0.0001921	Pa×s	552.02	Joback Method
dvisc	0.0003822	Pa×s	490.71	Joback Method
dvisc	0.0009255	Pa×s	429.40	Joback Method
dvisc	0.0030090	Pa×s	368.09	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=U361804&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