Malonic acid, di(4-methylpent-2-yl) ester

Other names: di-(1,3-Dimethylbutyl)malonate
Inchi: InChI=1S/C15H28O4/c1-10(2)7-12(5)18-14(16)9-15(17)19-13(6)8-11(3)4/h10-13H,7-9H2
InchiKey: PJQUZCUGAQDHHI-UHFFFAOYSA-N
Formula: C15H28O4
SMILES: CC(C)CC(C)OC(=O)CC(=O)OC(C)CC(C)C
Mol. weight [g/mol]: 272.38

Physical Properties

Property code	Value	Unit	Source
gf	-402.18	kJ/mol	Joback Method
hf	-863.65	kJ/mol	Joback Method
hfus	26.09	kJ/mol	Joback Method
hvap	65.74	kJ/mol	Joback Method
log10ws	-3.57		Crippen Method
logp	3.332		Crippen Method
mcvol	237.090	ml/mol	McGowan Method
pc	1557.35	kPa	Joback Method
rinpol	1575.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1575.00		NIST Webbook
tb	693.42	K	Joback Method
tc	878.58	K	Joback Method
tf	343.13	K	Joback Method
vc	0.899	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	679.17	J/mol×K	693.42	Joback Method
cpg	696.25	J/mol×K	724.28	Joback Method
cpg	712.44	J/mol×K	755.14	Joback Method
cpg	727.76	J/mol×K	786.00	Joback Method
cpg	742.20	J/mol×K	816.86	Joback Method
cpg	755.78	J/mol×K	847.72	Joback Method

cpg	768.51	J/mol×K	878.58	Joback Method
dvisc	0.0036197	Pa×s	343.13	Joback Method
dvisc	0.0011973	Pa×s	401.51	Joback Method
dvisc	0.0005245	Pa×s	459.89	Joback Method
dvisc	0.0002767	Pa×s	518.27	Joback Method
dvisc	0.0001662	Pa×s	576.66	Joback Method
dvisc	0.0001096	Pa×s	635.04	Joback Method
dvisc	0.0000775	Pa×s	693.42	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=U349346&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

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