

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:	RXSGWLRXFBPEEO-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
mvol	265.270	ml/mol	McGowan Method
pc	1364.66	kPa	Joback Method
rinpol	1740.00		NIST Webbook
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tb	735.95	K	Joback Method
tc	926.53	K	Joback Method
tf	368.09	K	Joback Method
vc	1.000	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.79	J/molxK	735.95	Joback Method
cpg	812.89	J/molxK	767.71	Joback Method
cpg	829.94	J/molxK	799.48	Joback Method
cpg	845.97	J/molxK	831.24	Joback Method
cpg	861.00	J/molxK	863.00	Joback Method
cpg	875.06	J/molxK	894.77	Joback Method
cpg	888.18	J/molxK	926.53	Joback Method
dvisc	0.0030090	Paxs	368.09	Joback Method

dvisc	0.0009255	Paxs	429.40	Joback Method
dvisc	0.0003822	Paxs	490.71	Joback Method
dvisc	0.0001921	Paxs	552.02	Joback Method
dvisc	0.0001108	Paxs	613.33	Joback Method
dvisc	0.0000706	Paxs	674.64	Joback Method
dvisc	0.0000485	Paxs	735.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361804&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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