

Dimethylmalonic acid, di(2-methylphenyl) ester

Inchi:	InChI=1S/C19H20O4/c1-13-9-5-7-11-15(13)22-17(20)19(3,4)18(21)23-16-12-8-6-10-14(1)
InchiKey:	WIKFZBYOZGEOMF-UHFFFAOYSA-N
Formula:	C19H20O4
SMILES:	Cc1ccccc1OC(=O)C(C)(C)C(=O)Oc1ccccc1C
Mol. weight [g/mol]:	312.36

Physical Properties

Property code	Value	Unit	Source
gf	-150.34	kJ/mol	Joback Method
hf	-483.72	kJ/mol	Joback Method
hfus	30.43	kJ/mol	Joback Method
hvap	80.78	kJ/mol	Joback Method
log10ws	-4.88		Crippen Method
logp	3.841		Crippen Method
mcvol	245.930	ml/mol	McGowan Method
pc	1892.00	kPa	Joback Method
rinpol	2183.00		NIST Webbook
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tb	846.79	K	Joback Method
tc	1083.08	K	Joback Method
tf	528.51	K	Joback Method
vc	0.920	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.55	J/molxK	846.79	Joback Method
cpg	783.40	J/molxK	1043.70	Joback Method
cpg	774.03	J/molxK	1004.31	Joback Method
cpg	763.51	J/molxK	964.93	Joback Method
cpg	751.80	J/molxK	925.55	Joback Method
cpg	738.83	J/molxK	886.17	Joback Method
cpg	791.69	J/molxK	1083.08	Joback Method
dvisc	0.0000514	Paxs	846.79	Joback Method

dvisc	0.0000654	Paxs	793.74	Joback Method
dvisc	0.0000860	Paxs	740.70	Joback Method
dvisc	0.0001180	Paxs	687.65	Joback Method
dvisc	0.0001708	Paxs	634.60	Joback Method
dvisc	0.0002644	Paxs	581.56	Joback Method
dvisc	0.0004469	Paxs	528.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361912&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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