Dimethylmalonic acid, di(3-methylphenyl) ester

Inchi: InChI=1S/C19H20O4/c1-13-7-5-9-15(11-13)22-17(20)19(3,4)18(21)23-16-10-6-8-14(2)12

InchiKey: UQSYKRWPYWYPID-UHFFFAOYSA-N

Formula: C19H20O4

SMILES: Cc1cccc(OC(=O)C(C)(C)C(=O)Oc2cccc(C)c2)c1

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	2211.00		NIST Webbook
tb	846.79	K	Joback Method
tc	1083.08	K	Joback Method
tf	528.51	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	724.55	J/mol×K	846.79	Joback Method
cpg	738.83	J/mol×K	886.17	Joback Method
cpg	751.80	J/mol×K	925.55	Joback Method
cpg	763.51	J/mol×K	964.93	Joback Method
cpg	774.03	J/mol×K	1004.31	Joback Method
cpg	783.40	J/mol×K	1043.70	Joback Method
cpg	791.69	J/mol×K	1083.08	Joback Method
dvisc	0.0004469	Pa×s	528.51	Joback Method
dvisc	0.0002644	Pa×s	581.56	Joback Method

dvisc	0.0001708	Pa×s	634.60	Joback Method
dvisc	0.0001180	Pa×s	687.65	Joback Method
dvisc	0.0000860	Pa×s	740.70	Joback Method
dvisc	0.0000654	Pa×s	793.74	Joback Method
dvisc	0.0000514	Pa×s	846.79	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=U363618&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