Dimethylmalonic acid, di(2,3,4-trifluorophenyl) ester

Inchi: InChI=1S/C17H10F6O4/c1-17(2,15(24)26-9-5-3-7(18)11(20)13(9)22)16(25)27-10-6-4-8(1

InchiKey: NXSIWYZUHCJLPI-UHFFFAOYSA-N

Formula: C17H10F6O4

SMILES: CC(C)(C(=O)Oc1ccc(F)c(F)c1F)C(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 392.25

Physical Properties

Property code	Value	Unit	Source
gf	-1374.56	kJ/mol	Joback Method
hf	-1664.98	kJ/mol	Joback Method
hfus	42.17	kJ/mol	Joback Method
hvap	74.07	kJ/mol	Joback Method
log10ws	-5.91		Crippen Method
logp	4.058		Crippen Method
mcvol	228.370	ml/mol	McGowan Method
pc	1683.79	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	816.57	K	Joback Method
tc	1018.95	K	Joback Method
tf	559.59	K	Joback Method
vc	0.916	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	653.35	J/mol×K	816.57	Joback Method
cpg	663.87	J/mol×K	850.30	Joback Method
cpg	673.50	J/mol×K	884.03	Joback Method
cpg	682.25	J/mol×K	917.76	Joback Method
cpg	690.14	J/mol×K	951.49	Joback Method
cpg	697.18	J/mol×K	985.22	Joback Method
cpg	703.40	J/mol×K	1018.95	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U361897&Units=SI

Legend

cpg:	Ideal gas heat capacity
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