Dimethylmalonic acid, di(3,5-difluorophenyl) ester

Inchi: InChI=1S/C17H12F4O4/c1-17(2,15(22)24-13-5-9(18)3-10(19)6-13)16(23)25-14-7-11(20)
InchiKey: ODECUYAWTNPSDR-UHFFFAOYSA-N
Formula: C17H12F4O4
SMILES: CC(C)(C(=O)Oc1cc(F)cc(F)c1)C(=O)Oc1cc(F)cc(F)c1
Mol. weight [g/mol]: 356.27

Physical Properties

Property code	Value	Unit	Source
gf	-965.68	kJ/mol	Joback Method
hf	-1249.82	kJ/mol	Joback Method
hfus	36.79	kJ/mol	Joback Method
hvap	74.38	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.780		Crippen Method
mcvol	224.830	ml/mol	McGowan Method
pc	1862.72	kPa	Joback Method
rinpol	1810.00		NIST Webbook
rinpol	1810.00		NIST Webbook
tb	808.07	K	Joback Method
tc	1020.74	K	Joback Method
tf	533.37	K	Joback Method
vc	0.880	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.10	J/mol×K	808.07	Joback Method
cpg	652.62	J/mol×K	843.51	Joback Method
cpg	663.14	J/mol×K	878.96	Joback Method
cpg	672.70	J/mol×K	914.40	Joback Method
cpg	681.31	J/mol×K	949.85	Joback Method
cpg	689.01	J/mol×K	985.29	Joback Method
cpg	695.84	J/mol×K	1020.74	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=U361816&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