Dimethylmalonic acid, isohexyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H21F3O4/c1-10(2)6-5-9-23-15(21)17(3,4)16(22)24-12-8-7-11(18)13(19)14

InchiKey: BQGWLJHVUFOEAS-UHFFFAOYSA-N

Formula: C17H21F3O4

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

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-876.09	kJ/mol	Joback Method
hf	-1284.05	kJ/mol	Joback Method
hfus	36.54	kJ/mol	Joback Method
hvap	71.88	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	4.015		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1502.31	kPa	Joback Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		NIST Webbook
tb	776.70	K	Joback Method
tc	970.93	K	Joback Method
tf	478.84	K	Joback Method
vc	0.965	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.03	J/mol×K	776.70	Joback Method
cpg	742.14	J/mol×K	809.07	Joback Method
cpg	755.31	J/mol×K	841.44	Joback Method
cpg	767.57	J/mol×K	873.81	Joback Method
cpg	778.93	J/mol×K	906.18	Joback Method
cpg	789.41	J/mol×K	938.55	Joback Method
cpg	799.04	J/mol×K	970.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361884&Units=SI
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

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