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

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

InchiKey: CPJDZQLJOCBUTQ-UHFFFAOYSA-N

Formula: C17H21F3O4

SMILES: CCCCCCOC(=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	-873.65	kJ/mol	Joback Method
hf	-1278.77	kJ/mol	Joback Method
hfus	40.06	kJ/mol	Joback Method
hvap	72.26	kJ/mol	Joback Method
log10ws	-5.17		Crippen Method
logp	4.159		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	1856.00		NIST Webbook
tb	777.14	K	Joback Method
tc	969.24	K	Joback Method
tf	493.84	K	Joback Method
vc	0.971	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	727.48	J/mol×K	777.14	Joback Method
cpg	741.43	J/mol×K	809.16	Joback Method
cpg	754.47	J/mol×K	841.17	Joback Method
cpg	766.63	J/mol×K	873.19	Joback Method
cpg	777.92	J/mol×K	905.21	Joback Method
cpg	788.36	J/mol×K	937.23	Joback Method
cpg	797.97	J/mol×K	969.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361885&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