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

Inchi: InChI=1S/C14H15F3O4/c1-4-7-20-12(18)14(2,3)13(19)21-9-6-5-8(15)10(16)11(9)17/h5-6

InchiKey: JVALGMNLDYMAPK-UHFFFAOYSA-N

Formula: C14H15F3O4

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

Mol. weight [g/mol]: 304.26

Physical Properties

Property code	Value	Unit	Source
gf	-898.91	kJ/mol	Joback Method
hf	-1216.85	kJ/mol	Joback Method
hfus	32.29	kJ/mol	Joback Method
hvap	65.59	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	2.989		Crippen Method
mcvol	204.550	ml/mol	McGowan Method
pc	1890.36	kPa	Joback Method
rinpol	1584.00		NIST Webbook
rinpol	1584.00		NIST Webbook
tb	708.50	K	Joback Method
tc	902.90	K	Joback Method
tf	460.03	K	Joback Method
vc	0.802	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.45	J/mol×K	708.50	Joback Method
cpg	577.20	J/mol×K	740.90	Joback Method
cpg	589.16	J/mol×K	773.30	Joback Method
cpg	600.34	J/mol×K	805.70	Joback Method
cpg	610.74	J/mol×K	838.10	Joback Method
cpg	620.39	J/mol×K	870.50	Joback Method
cpg	629.30	J/mol×K	902.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361881&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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