Dimethylmalonic acid, ethyl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C14H14F4O4/c1-4-21-11(19)13(2,3)12(20)22-9-7-5-6-8(10(9)15)14(16,17)18/h

InchiKey: FGCGNCIXHANHBY-UHFFFAOYSA-N

Formula: C14H14F4O4

SMILES: CCOC(=O)C(C)(C)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 322.25

Physical Properties

Property code	Value	Unit	Source
gf	-1081.25	kJ/mol	Joback Method
hf	-1410.24	kJ/mol	Joback Method
hfus	28.35	kJ/mol	Joback Method
hvap	62.81	kJ/mol	Joback Method
log10ws	-3.93		Crippen Method
logp	3.339		Crippen Method
mcvol	206.320	ml/mol	McGowan Method
pc	1872.41	kPa	Joback Method
rinpol	1510.00		NIST Webbook
rinpol	1510.00		NIST Webbook
tb	699.56	K	Joback Method
tc	894.51	K	Joback Method
tf	450.52	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	576.13	J/mol×K	699.56	Joback Method
cpg	588.79	J/mol×K	732.05	Joback Method
cpg	600.59	J/mol×K	764.54	Joback Method
cpg	611.54	J/mol×K	797.03	Joback Method
cpg	621.70	J/mol×K	829.53	Joback Method
cpg	631.09	J/mol×K	862.02	Joback Method
cpg	639.75	J/mol×K	894.51	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361995&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