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

Inchi: InChI=1S/C17H20F4O4/c1-4-5-6-10-24-14(22)16(2,3)15(23)25-12-9-7-8-11(13(12)18)17

InchiKey: RFUKWHMVNPHKTF-UHFFFAOYSA-N

Formula: C17H20F4O4

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

Mol. weight [g/mol]: 364.33

Physical Properties

Property code	Value	Unit	Source
gf	-1055.99	kJ/mol	Joback Method
hf	-1472.16	kJ/mol	Joback Method
hfus	36.11	kJ/mol	Joback Method
hvap	69.49	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.510		Crippen Method
mcvol	248.590	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1770.00		NIST Webbook
tb	768.20	K	Joback Method
tc	960.27	K	Joback Method
tf	484.33	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	737.95	J/mol×K	768.20	Joback Method
cpg	751.69	J/mol×K	800.21	Joback Method
cpg	764.51	J/mol×K	832.22	Joback Method
cpg	776.43	J/mol×K	864.23	Joback Method
cpg	787.51	J/mol×K	896.25	Joback Method
cpg	797.77	J/mol×K	928.26	Joback Method
cpg	807.26	J/mol×K	960.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361997&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