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

Inchi: InChI=1S/C18H22F4O4/c1-11(2)7-6-10-25-15(23)17(3,4)16(24)26-13-9-5-8-12(14(13)19)18(20,21)22/h5,8-9,11H,6-7,10H2,1-4H3

InchiKey: HYPDVFWRDFLDTB-UHFFFAOYSA-N

Formula: C18H22F4O4

SMILES: CC(C)CCCOC(=O)C(C)(C)C(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 378.36

Physical Properties

Property code	Value	Unit	Source
gf	-1050.01	kJ/mol	Joback Method
hf	-1498.08	kJ/mol	Joback Method
hfus	35.18	kJ/mol	Joback Method
hvap	71.33	kJ/mol	Joback Method
log10ws	-5.37		Crippen Method
logp	4.756		Crippen Method
mcvol	262.680	ml/mol	McGowan Method
pc	1385.05	kPa	Joback Method
rinpol	1826.00		NIST Webbook
rinpol	1826.00		NIST Webbook
tb	790.64	K	Joback Method
tc	984.78	K	Joback Method
tf	480.60	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.51	J/mol×K	790.64	Joback Method
cpg	808.72	J/mol×K	823.00	Joback Method
cpg	821.94	J/mol×K	855.35	Joback Method
cpg	834.22	J/mol×K	887.71	Joback Method
cpg	845.60	J/mol×K	920.07	Joback Method
cpg	856.13	J/mol×K	952.42	Joback Method
cpg	865.85	J/mol×K	984.78	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U361998&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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