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

Inchi: InChI=1S/C20H26F4O4/c1-4-5-6-7-8-9-13-27-17(25)19(2,3)18(26)28-15-12-10-11-14(16

InchiKey: XJEHPPDNRCYMSC-UHFFFAOYSA-N

Formula: C20H26F4O4

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

Mol. weight [g/mol]: 406.41

Physical Properties

Property code	Value	Unit	Source
gf	-1030.73	kJ/mol	Joback Method
hf	-1534.08	kJ/mol	Joback Method
hfus	43.88	kJ/mol	Joback Method
hvap	76.17	kJ/mol	Joback Method
log10ws	-6.45		Crippen Method
logp	5.680		Crippen Method
mcvol	290.860	ml/mol	McGowan Method
pc	1199.79	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	836.84	K	Joback Method
tc	1031.26	K	Joback Method
tf	518.14	K	Joback Method
vc	1.145	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.69	J/mol×K	836.84	Joback Method
cpg	923.37	J/mol×K	869.24	Joback Method
cpg	937.03	J/mol×K	901.65	Joback Method
cpg	949.73	J/mol×K	934.05	Joback Method
cpg	961.51	J/mol×K	966.45	Joback Method
cpg	972.43	J/mol×K	998.85	Joback Method
cpg	982.53	J/mol×K	1031.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362000&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