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

Inchi: InChI=1S/C22H30F4O4/c1-4-5-6-7-8-9-10-11-15-29-19(27)21(2,3)20(28)30-17-14-12-13

InchiKey: WHHZNYUWMDQYCA-UHFFFAOYSA-N

Formula: C22H30F4O4

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

Mol. weight [g/mol]: 434.46

Physical Properties

Property code	Value	Unit	Source
gf	-1013.89	kJ/mol	Joback Method
hf	-1575.36	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	80.62	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	6.460		Crippen Method
mcvol	319.040	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook
tb	882.60	K	Joback Method
tc	1082.19	K	Joback Method
tf	540.68	K	Joback Method
vc	1.258	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.60	J/mol×K	882.60	Joback Method
cpg	1041.93	J/mol×K	915.87	Joback Method
cpg	1056.18	J/mol×K	949.13	Joback Method
cpg	1069.39	J/mol×K	982.40	Joback Method
cpg	1081.62	J/mol×K	1015.66	Joback Method
cpg	1092.95	J/mol×K	1048.93	Joback Method
cpg	1103.41	J/mol×K	1082.19	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U362002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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