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

Inchi: InChI=1S/C19H24F4O4/c1-4-7-8-12-26-16(24)18(5-2,6-3)17(25)27-14-11-9-10-13(15(14

InchiKey: BJTLIIBRCDTWLZ-UHFFFAOYSA-N

Formula: C19H24F4O4

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

Mol. weight [g/mol]: 392.39

Physical Properties

Property code	Value	Unit	Source
gf	-1039.15	kJ/mol	Joback Method
hf	-1513.44	kJ/mol	Joback Method
hfus	41.29	kJ/mol	Joback Method
hvap	73.94	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	5.290		Crippen Method
mcvol	276.770	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	1909.00		NIST Webbook
tb	813.96	K	Joback Method
tc	1006.93	K	Joback Method
tf	506.87	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.90	J/mol×K	813.96	Joback Method
cpg	865.26	J/mol×K	846.12	Joback Method
cpg	878.65	J/mol×K	878.28	Joback Method
cpg	891.10	J/mol×K	910.44	Joback Method
cpg	902.65	J/mol×K	942.60	Joback Method
cpg	913.36	J/mol×K	974.77	Joback Method
cpg	923.28	J/mol×K	1006.93	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=U370711&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