Diethylmalonic acid, hexyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C19H25F3O4/c1-4-7-8-9-12-25-17(23)19(5-2,6-3)18(24)26-14-11-10-13(20)15

InchiKey: BMLTVSLHAFVISG-UHFFFAOYSA-N

Formula: C19H25F3O4

SMILES: CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 374.39

Physical Properties

Property code	Value	Unit	Source
gf	-856.81	kJ/mol	Joback Method
hf	-1320.05	kJ/mol	Joback Method
hfus	45.24	kJ/mol	Joback Method
hvap	76.72	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	4.939		Crippen Method
mcvol	275.000	ml/mol	McGowan Method
pc	1293.93	kPa	Joback Method
rinpol	1989.00		NIST Webbook
rinpol	1989.00		NIST Webbook
tb	822.90	K	Joback Method
tc	1016.39	K	Joback Method
tf	516.38	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.26	J/mol×K	822.90	Joback Method
cpg	855.87	J/mol×K	855.15	Joback Method
cpg	869.48	J/mol×K	887.40	Joback Method
cpg	882.13	J/mol×K	919.64	Joback Method
cpg	893.85	J/mol×K	951.89	Joback Method
cpg	904.64	J/mol×K	984.14	Joback Method
cpg	914.55	J/mol×K	1016.39	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=U370692&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