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

Inchi: InChI=1S/C16H19F3O4/c1-4-9-22-14(20)16(5-2,6-3)15(21)23-11-8-7-10(17)12(18)13(11

InchiKey: LIQQNYMGGFIYPE-UHFFFAOYSA-N

Formula: C16H19F3O4

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

Mol. weight [g/mol]: 332.31

Physical Properties

Property code	Value	Unit	Source
gf	-882.07	kJ/mol	Joback Method
hf	-1258.13	kJ/mol	Joback Method
hfus	37.47	kJ/mol	Joback Method
hvap	70.04	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	3.769		Crippen Method
mcvol	232.730	ml/mol	McGowan Method
pc	1610.29	kPa	Joback Method
rinpol	1740.00		NIST Webbook
tb	754.26	K	Joback Method
tc	946.60	K	Joback Method
tf	482.57	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.04	J/mol×K	754.26	Joback Method
cpg	685.63	J/mol×K	786.32	Joback Method
cpg	698.35	J/mol×K	818.37	Joback Method
cpg	710.22	J/mol×K	850.43	Joback Method
cpg	721.25	J/mol×K	882.48	Joback Method
cpg	731.47	J/mol×K	914.54	Joback Method
cpg	740.89	J/mol×K	946.60	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=U370688&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