Diethylmalonic acid, di(2,3,4-trifluorophenyl) ester

Inchi: InChI=1S/C19H14F6O4/c1-3-19(4-2,17(26)28-11-7-5-9(20)13(22)15(11)24)18(27)29-12-
InchiKey: DNGLADCQRZZKGL-UHFFFAOYSA-N
Formula: C19H14F6O4
SMILES: CCC(CC)(C(=O)Oc1ccc(F)c(F)c1F)C(=O)Oc1ccc(F)c(F)c1F
Mol. weight [g/mol]: 420.30

Physical Properties

Property code	Value	Unit	Source
gf	-1357.72	kJ/mol	Joback Method
hf	-1706.26	kJ/mol	Joback Method
hfus	47.35	kJ/mol	Joback Method
hvap	78.53	kJ/mol	Joback Method
log10ws	-6.75		Crippen Method
logp	4.839		Crippen Method
mcvol	256.550	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		NIST Webbook
tb	862.33	K	Joback Method
tc	1065.47	K	Joback Method
tf	582.13	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	763.79	J/mol×K	862.33	Joback Method
cpg	774.96	J/mol×K	896.19	Joback Method
cpg	785.15	J/mol×K	930.04	Joback Method
cpg	794.38	J/mol×K	963.90	Joback Method
cpg	802.67	J/mol×K	997.76	Joback Method
cpg	810.06	J/mol×K	1031.61	Joback Method
cpg	816.55	J/mol×K	1065.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370704&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