Diethylmalonic acid, isobutyl 2,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C18H23F3O4/c1-5-18(6-2,16(22)24-9-11(3)4)17(23)25-10-12-7-14(20)15(21)8

InchiKey: LGEOTRXUOIMZRH-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCC(CC)(C(=O)OCc1cc(F)c(F)cc1F)C(=O)OCC(C)C

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-867.67	kJ/mol	Joback Method
hf	-1304.69	kJ/mol	Joback Method
hfus	39.13	kJ/mol	Joback Method
hvap	74.10	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	4.153		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1396.46	kPa	Joback Method
rinpol	1864.00		NIST Webbook
tb	799.58	K	Joback Method
tc	993.88	K	Joback Method
tf	490.11	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.46	J/mol×K	799.58	Joback Method
cpg	798.88	J/mol×K	831.96	Joback Method
cpg	812.32	J/mol×K	864.35	Joback Method
cpg	824.82	J/mol×K	896.73	Joback Method
cpg	836.38	J/mol×K	929.11	Joback Method
cpg	847.04	J/mol×K	961.49	Joback Method
cpg	856.82	J/mol×K	993.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369256&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