Diethylmalonic acid, butyl 3,4,5-trifluorobenzyl ester

Inchi: InChI=1S/C18H23F3O4/c1-4-7-8-24-16(22)18(5-2,6-3)17(23)25-11-12-9-13(19)15(21)14

InchiKey: QDEUAWFCQAKLEJ-UHFFFAOYSA-N

Formula: C18H23F3O4

SMILES: CCCCOC(=O)C(CC)(CC)C(=O)OCc1cc(F)c(F)c(F)c1

Mol. weight [g/mol]: 360.37

Physical Properties

Property code	Value	Unit	Source
gf	-865.23	kJ/mol	Joback Method
hf	-1299.41	kJ/mol	Joback Method
hfus	42.65	kJ/mol	Joback Method
hvap	74.49	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	4.297		Crippen Method
mcvol	260.910	ml/mol	McGowan Method
pc	1388.15	kPa	Joback Method
rinpol	1922.00		NIST Webbook
tb	800.02	K	Joback Method
tc	992.49	K	Joback Method
tf	505.11	K	Joback Method
vc	1.026	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.91	J/mol×K	800.02	Joback Method
cpg	798.20	J/mol×K	832.10	Joback Method
cpg	811.54	J/mol×K	864.18	Joback Method
cpg	823.95	J/mol×K	896.26	Joback Method
cpg	835.46	J/mol×K	928.33	Joback Method
cpg	846.09	J/mol×K	960.41	Joback Method
cpg	855.87	J/mol×K	992.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369273&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

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