Diethylmalonic acid, di(3,4,5-trifluorobenzyl) ester

Inchi: InChI=1S/C21H18F6O4/c1-3-21(4-2,19(28)30-9-11-5-13(22)17(26)14(23)6-11)20(29)31-

InchiKey: WCHFANIAFSUGEG-UHFFFAOYSA-N

Formula: C21H18F6O4

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

Mol. weight [g/mol]: 448.36

Physical Properties

Property code	Value	Unit	Source
gf	-1340.88	kJ/mol	Joback Method
hf	-1747.54	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	82.98	kJ/mol	Joback Method
log10ws	-7.28		Crippen Method
logp	5.114		Crippen Method
mcvol	284.730	ml/mol	McGowan Method
pc	1256.59	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	908.09	K	Joback Method
tc	1114.98	K	Joback Method
tf	604.67	K	Joback Method
vc	1.141	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	877.47	J/mol×K	908.09	Joback Method
cpg	889.21	J/mol×K	942.57	Joback Method
cpg	899.87	J/mol×K	977.05	Joback Method
cpg	909.47	J/mol×K	1011.54	Joback Method
cpg	918.05	J/mol×K	1046.02	Joback Method
cpg	925.63	J/mol×K	1080.50	Joback Method
cpg	932.24	J/mol×K	1114.98	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369274&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