Diethylmalonic acid, ethyl 4-trifluoromethylbenzyl ester

Inchi: InChI=1S/C17H21F3O4/c1-4-16(5-2,14(21)23-6-3)15(22)24-11-12-7-9-13(10-8-12)17(18

InchiKey: USMAWAWQDRDIJE-UHFFFAOYSA-N

Formula: C17H21F3O4

SMILES: CCOC(=O)C(CC)(CC)C(=O)OCc1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 346.34

Physical Properties

Property code	Value	Unit	Source
gf	-851.55	kJ/mol	Joback Method
hf	-1264.58	kJ/mol	Joback Method
hfus	33.42	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.118		Crippen Method
mcvol	246.820	ml/mol	McGowan Method
pc	1551.22	kPa	Joback Method
rinpol	1787.00		NIST Webbook
rinpol	1787.00		NIST Webbook
tb	763.95	K	Joback Method
tc	960.67	K	Joback Method
tf	471.22	K	Joback Method
vc	0.960	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.15	J/mol×K	763.95	Joback Method
cpg	745.48	J/mol×K	796.74	Joback Method
cpg	758.81	J/mol×K	829.52	Joback Method
cpg	771.20	J/mol×K	862.31	Joback Method
cpg	782.70	J/mol×K	895.10	Joback Method
cpg	793.34	J/mol×K	927.88	Joback Method
cpg	803.18	J/mol×K	960.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368399&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