Diethylmalonic acid, 3,4-difluorobenzyl propyl ester

Inchi: InChI=1S/C17H22F2O4/c1-4-9-22-15(20)17(5-2,6-3)16(21)23-11-12-7-8-13(18)14(19)10

InchiKey: GRWXCDAWROEIEP-UHFFFAOYSA-N

Formula: C17H22F2O4

SMILES: CCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(F)c(F)c1

Mol. weight [g/mol]: 328.35

Physical Properties

Property code	Value	Unit	Source
gf	-669.21	kJ/mol	Joback Method
hf	-1071.19	kJ/mol	Joback Method
hfus	37.37	kJ/mol	Joback Method
hvap	72.42	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.768		Crippen Method
mcvol	245.050	ml/mol	McGowan Method
pc	1564.75	kPa	Joback Method
rinpol	1876.00		NIST Webbook
rinpol	1876.00		NIST Webbook
tb	772.89	K	Joback Method
tc	969.40	K	Joback Method
tf	480.73	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.69	J/mol×K	772.89	Joback Method
cpg	735.20	J/mol×K	805.64	Joback Method
cpg	748.75	J/mol×K	838.39	Joback Method
cpg	761.37	J/mol×K	871.14	Joback Method
cpg	773.07	J/mol×K	903.89	Joback Method
cpg	783.89	J/mol×K	936.65	Joback Method
cpg	793.86	J/mol×K	969.40	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369323&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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