Diethylmalonic acid, 4-fluoro-2-methoxyphenyl propyl ester

Inchi: InChI=1S/C17H23FO5/c1-5-10-22-15(19)17(6-2,7-3)16(20)23-13-9-8-12(18)11-14(13)21

InchiKey: VJRXUUOEUSKXQJ-UHFFFAOYSA-N

Formula: C17H23FO5

SMILES: CCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 326.36

Physical Properties

Property code	Value	Unit	Source
gf	-579.40	kJ/mol	Joback Method
hf	-1007.30	kJ/mol	Joback Method
hfus	35.48	kJ/mol	Joback Method
hvap	75.64	kJ/mol	Joback Method
log10ws	-4.21		Crippen Method
logp	3.499		Crippen Method
mcvol	249.150	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2004.00		NIST Webbook
rinpol	2004.00		NIST Webbook
tb	796.04	K	Joback Method
tc	998.12	K	Joback Method
tf	502.37	K	Joback Method
vc	0.953	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	741.04	J/mol×K	796.04	Joback Method
cpg	755.66	J/mol×K	829.72	Joback Method
cpg	769.24	J/mol×K	863.40	Joback Method
cpg	781.78	J/mol×K	897.08	Joback Method
cpg	793.30	J/mol×K	930.76	Joback Method
cpg	803.82	J/mol×K	964.44	Joback Method
cpg	813.34	J/mol×K	998.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370880&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