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

Inchi: InChI=1S/C19H27FO5/c1-5-8-9-12-24-17(21)19(6-2,7-3)18(22)25-15-11-10-14(20)13-16

InchiKey: PKUIGTWTFLUFNU-UHFFFAOYSA-N

Formula: C19H27FO5

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

Mol. weight [g/mol]: 354.41

Physical Properties

Property code	Value	Unit	Source
gf	-562.56	kJ/mol	Joback Method
hf	-1048.58	kJ/mol	Joback Method
hfus	40.66	kJ/mol	Joback Method
hvap	80.10	kJ/mol	Joback Method
log10ws	-5.04		Crippen Method
logp	4.279		Crippen Method
mcvol	277.330	ml/mol	McGowan Method
pc	1379.91	kPa	Joback Method
rinpol	2165.00		NIST Webbook
rinpol	2165.00		NIST Webbook
tb	841.80	K	Joback Method
tc	1043.63	K	Joback Method
tf	524.91	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	855.87	J/mol×K	841.80	Joback Method
cpg	870.94	J/mol×K	875.44	Joback Method
cpg	884.87	J/mol×K	909.08	Joback Method
cpg	897.69	J/mol×K	942.72	Joback Method
cpg	909.42	J/mol×K	976.36	Joback Method
cpg	920.08	J/mol×K	1009.99	Joback Method
cpg	929.69	J/mol×K	1043.63	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370883&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