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

Inchi: InChI=1S/C18H25FO5/c1-6-18(7-2,16(20)23-11-12(3)4)17(21)24-14-9-8-13(19)10-15(14

InchiKey: KEZXHLPWUURWGX-UHFFFAOYSA-N

Formula: C18H25FO5

SMILES: CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 340.39

Physical Properties

Property code	Value	Unit	Source
gf	-573.42	kJ/mol	Joback Method
hf	-1033.22	kJ/mol	Joback Method
hfus	34.54	kJ/mol	Joback Method
hvap	77.48	kJ/mol	Joback Method
log10ws	-4.38		Crippen Method
logp	3.745		Crippen Method
mcvol	263.240	ml/mol	McGowan Method
pc	1493.04	kPa	Joback Method
rinpol	2046.00		NIST Webbook
tb	818.48	K	Joback Method
tc	1022.30	K	Joback Method
tf	498.64	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.57	J/mol×K	818.48	Joback Method
cpg	813.58	J/mol×K	852.45	Joback Method
cpg	827.47	J/mol×K	886.42	Joback Method
cpg	840.25	J/mol×K	920.39	Joback Method
cpg	851.94	J/mol×K	954.36	Joback Method
cpg	862.57	J/mol×K	988.33	Joback Method
cpg	872.14	J/mol×K	1022.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370881&Units=SI

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

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