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

Inchi: InChI=1S/C18H25FO5/c1-5-8-11-23-16(20)18(6-2,7-3)17(21)24-14-10-9-13(19)12-15(14

InchiKey: AZMZSPAXYZMXGU-UHFFFAOYSA-N

Formula: C18H25FO5

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

Mol. weight [g/mol]: 340.39

Physical Properties

Property code	Value	Unit	Source
gf	-570.98	kJ/mol	Joback Method
hf	-1027.94	kJ/mol	Joback Method
hfus	38.07	kJ/mol	Joback Method
hvap	77.87	kJ/mol	Joback Method
log10ws	-4.62		Crippen Method
logp	3.889		Crippen Method
mcvol	263.240	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	2084.00		NIST Webbook
rinpol	2084.00		NIST Webbook
tb	818.92	K	Joback Method
tc	1020.55	K	Joback Method
tf	513.64	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	798.03	J/mol×K	818.92	Joback Method
cpg	812.88	J/mol×K	852.52	Joback Method
cpg	826.65	J/mol×K	886.13	Joback Method
cpg	839.35	J/mol×K	919.73	Joback Method
cpg	850.99	J/mol×K	953.34	Joback Method
cpg	861.59	J/mol×K	986.94	Joback Method
cpg	871.17	J/mol×K	1020.55	Joback Method

Sources

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=U370882&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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