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

Inchi: InChI=1S/C20H29FO5/c1-5-8-9-10-13-25-18(22)20(6-2,7-3)19(23)26-16-12-11-15(21)14

InchiKey: ZGGLXTPQIQFBIG-UHFFFAOYSA-N

Formula: C20H29FO5

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

Mol. weight [g/mol]: 368.44

Physical Properties

Property code	Value	Unit	Source
gf	-554.14	kJ/mol	Joback Method
hf	-1069.22	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	82.32	kJ/mol	Joback Method
log10ws	-5.46		Crippen Method
logp	4.670		Crippen Method
mcvol	291.420	ml/mol	McGowan Method
pc	1286.51	kPa	Joback Method
rinpol	2254.00		NIST Webbook
tb	864.68	K	Joback Method
tc	1067.42	K	Joback Method
tf	536.18	K	Joback Method
vc	1.121	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	914.50	J/mol×K	864.68	Joback Method
cpg	929.76	J/mol×K	898.47	Joback Method
cpg	943.84	J/mol×K	932.26	Joback Method
cpg	956.77	J/mol×K	966.05	Joback Method
cpg	968.56	J/mol×K	999.84	Joback Method
cpg	979.25	J/mol×K	1033.63	Joback Method
cpg	988.84	J/mol×K	1067.42	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=U370884&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