Diethylmalonic acid, di(4-fluoro-2-methoxyphenyl) ester

Inchi: InChI=1S/C21H22F2O6/c1-5-21(6-2,19(24)28-15-9-7-13(22)11-17(15)26-3)20(25)29-16-

InchiKey: BQNRXXKLOKNMNX-UHFFFAOYSA-N

Formula: C21H22F2O6

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

Mol. weight [g/mol]: 408.39

Physical Properties

Property code	Value	Unit	Source
gf	-752.38	kJ/mol	Joback Method
hf	-1204.60	kJ/mol	Joback Method
hfus	43.37	kJ/mol	Joback Method
hvap	89.74	kJ/mol	Joback Method
log10ws	-5.66		Crippen Method
logp	4.299		Crippen Method
mcvol	289.390	ml/mol	McGowan Method
pc	1429.38	kPa	Joback Method
rinpol	2524.00		NIST Webbook
tb	945.89	K	Joback Method
tc	1167.46	K	Joback Method
tf	621.73	K	Joback Method
vc	1.105	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	904.50	J/mol×K	945.89	Joback Method
cpg	916.22	J/mol×K	982.82	Joback Method
cpg	926.48	J/mol×K	1019.75	Joback Method
cpg	935.31	J/mol×K	1056.67	Joback Method
cpg	942.72	J/mol×K	1093.60	Joback Method
cpg	948.72	J/mol×K	1130.53	Joback Method
cpg	953.31	J/mol×K	1167.46	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370908&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