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

Inchi: InChI=1S/C21H31FO5/c1-5-8-9-10-11-14-26-19(23)21(6-2,7-3)20(24)27-17-13-12-16(22

InchiKey: NOZNEOOMOQEIBJ-UHFFFAOYSA-N

Formula: C21H31FO5

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

Mol. weight [g/mol]: 382.47

Physical Properties

Property code	Value	Unit	Source
gf	-545.72	kJ/mol	Joback Method
hf	-1089.86	kJ/mol	Joback Method
hfus	45.84	kJ/mol	Joback Method
hvap	84.55	kJ/mol	Joback Method
log10ws	-5.88		Crippen Method
logp	5.060		Crippen Method
mcvol	305.510	ml/mol	McGowan Method
pc	1202.29	kPa	Joback Method
rinpol	2346.00		NIST Webbook
tb	887.56	K	Joback Method
tc	1091.96	K	Joback Method
tf	547.45	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.84	J/mol×K	887.56	Joback Method
cpg	989.29	J/mol×K	921.63	Joback Method
cpg	1003.51	J/mol×K	955.69	Joback Method
cpg	1016.53	J/mol×K	989.76	Joback Method
cpg	1028.36	J/mol×K	1023.83	Joback Method
cpg	1039.04	J/mol×K	1057.90	Joback Method
cpg	1048.59	J/mol×K	1091.96	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=U370886&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