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

Inchi: InChI=1S/C22H33FO5/c1-5-8-9-10-11-12-15-27-20(24)22(6-2,7-3)21(25)28-18-14-13-17

InchiKey: BFARZKQPTJCKSD-UHFFFAOYSA-N

Formula: C22H33FO5

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

Mol. weight [g/mol]: 396.49

Physical Properties

Property code	Value	Unit	Source
gf	-537.30	kJ/mol	Joback Method
hf	-1110.50	kJ/mol	Joback Method
hfus	48.43	kJ/mol	Joback Method
hvap	86.77	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	5.450		Crippen Method
mcvol	319.600	ml/mol	McGowan Method
pc	1126.08	kPa	Joback Method
rinpol	2441.00		NIST Webbook
tb	910.44	K	Joback Method
tc	1117.32	K	Joback Method
tf	558.72	K	Joback Method
vc	1.232	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.83	J/mol×K	910.44	Joback Method
cpg	1049.47	J/mol×K	944.92	Joback Method
cpg	1063.83	J/mol×K	979.40	Joback Method
cpg	1076.92	J/mol×K	1013.88	Joback Method
cpg	1088.78	J/mol×K	1048.36	Joback Method
cpg	1099.43	J/mol×K	1082.84	Joback Method
cpg	1108.91	J/mol×K	1117.32	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370887&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

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