Glutaric acid, dec-2-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C22H33FO5/c1-4-5-6-7-8-9-11-17(2)27-21(24)12-10-13-22(25)28-19-15-14-18

InchiKey: ZMLUFKONIAXFQC-UHFFFAOYSA-N

Formula: C22H33FO5

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 396.49

Physical Properties

Property code	Value	Unit	Source
hfus	55.48	kJ/mol	Joback Method
logp	5.592		Crippen Method
mcvol	319.600	ml/mol	McGowan Method
rinpol	2598.00		NIST Webbook
rinpol	2598.00		NIST Webbook
tb	650.63	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	$Y = A + B \cdot T + C \cdot T^2 + D \cdot T^3 + E \cdot T.$
Y unit	J/mol×K
Coeff. A	5.83100e+01
Coeff. B	1.74086e+00
Coeff. C	-7.89520e-04
Coeff. D	6.24000e-08
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393449&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature

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