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
gf	-542.58	kJ/mol	Joback Method
hf	-1107.03	kJ/mol	Joback Method
hfus	52.32	kJ/mol	Joback Method
hvap	87.68	kJ/mol	Joback Method
log10ws	-6.65		Crippen Method
logp	5.592		Crippen Method
mcvol	319.600	ml/mol	McGowan Method
pc	1117.81	kPa	Joback Method
rinpol	2598.00		NIST Webbook
rinpol	2598.00		NIST Webbook
tb	913.23	K	Joback Method
tc	1119.27	K	Joback Method
tf	541.30	K	Joback Method
vc	1.238	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1033.89	J/mol×K	913.23	Joback Method
cpg	1049.57	J/mol×K	947.57	Joback Method
cpg	1063.88	J/mol×K	981.91	Joback Method
cpg	1076.83	J/mol×K	1016.25	Joback Method
cpg	1088.44	J/mol×K	1050.59	Joback Method
cpg	1098.72	J/mol×K	1084.93	Joback Method
cpg	1107.67	J/mol×K	1119.27	Joback Method

Sources

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=U393449&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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