Glutaric acid, dodec-2-en-1-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C24H35FO5/c1-3-4-5-6-7-8-9-10-11-12-18-29-23(26)14-13-15-24(27)30-21-17

InchiKey: KLLZUTBKYOZTLV-VAWYXSNFSA-N

Formula: C24H35FO5

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 422.53

Physical Properties

Property code	Value	Unit	Source
gf	-443.08	kJ/mol	Joback Method
hf	-1025.81	kJ/mol	Joback Method
hfus	61.22	kJ/mol	Joback Method
hvap	92.48	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.150		Crippen Method
mcvol	343.480	ml/mol	McGowan Method
pc	1014.89	kPa	Joback Method
rinpol	2915.00		NIST Webbook
rinpol	2915.00		NIST Webbook
tb	963.59	K	Joback Method
tc	1179.72	K	Joback Method
tf	573.76	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1127.03	J/mol×K	963.59	Joback Method
cpg	1142.77	J/mol×K	999.61	Joback Method
cpg	1157.09	J/mol×K	1035.63	Joback Method
cpg	1170.02	J/mol×K	1071.66	Joback Method
cpg	1181.60	J/mol×K	1107.68	Joback Method
cpg	1191.86	J/mol×K	1143.70	Joback Method
cpg	1200.83	J/mol×K	1179.72	Joback Method

Sources

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=U393453&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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