Glutaric acid, dodec-2-en-1-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C23H31F3O4/c1-2-3-4-5-6-7-8-9-10-11-17-29-20(27)13-12-14-21(28)30-19-16-15-18(24)22(25)23(19)26

InchiKey: BHMVHTWFRVLJDW-ZHACJKMWSA-N

Formula: C23H31F3O4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 428.49

Physical Properties

Property code	Value	Unit	Source
gf	-745.75	kJ/mol	Joback Method
hf	-1276.64	kJ/mol	Joback Method
hfus	63.22	kJ/mol	Joback Method
hvap	86.87	kJ/mol	Joback Method
log10ws	-7.78		Crippen Method
logp	6.420		Crippen Method
mcvol	327.060	ml/mol	McGowan Method
pc	1020.08	kPa	Joback Method
rinpol	2695.00		NIST Webbook
rinpol	2695.00		NIST Webbook
tb	921.81	K	Joback Method
tc	1128.55	K	Joback Method
tf	553.96	K	Joback Method
vc	1.298	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1050.30	J/mol×K	921.81	Joback Method
cpg	1065.88	J/mol×K	956.27	Joback Method
cpg	1080.27	J/mol×K	990.72	Joback Method
cpg	1093.50	J/mol×K	1025.18	Joback Method
cpg	1105.62	J/mol×K	1059.64	Joback Method
cpg	1116.66	J/mol×K	1094.10	Joback Method
cpg	1126.66	J/mol×K	1128.55	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=U393648&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