Glutaric acid, dodec-2-en-1-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C24H32F4O4/c1-2-3-4-5-6-7-8-9-10-11-18-31-21(29)16-13-17-22(30)32-20-15

InchiKey: OQUIGVPURKNMDF-ZHACJKMWSA-N

Formula: C24H32F4O4

SMILES: CCCCCCCCCC=CCOC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 460.50

Physical Properties

Property code	Value	Unit	Source
gf	-919.67	kJ/mol	Joback Method
hf	-1490.67	kJ/mol	Joback Method
hfus	61.86	kJ/mol	Joback Method
hvap	86.32	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.160		Crippen Method
mcvol	342.920	ml/mol	McGowan Method
pc	953.78	kPa	Joback Method
rinpol	2684.00		NIST Webbook
rinpol	2684.00		NIST Webbook
tb	935.75	K	Joback Method
tc	1145.84	K	Joback Method
tf	555.72	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.01	J/mol×K	935.75	Joback Method
cpg	1134.81	J/mol×K	970.76	Joback Method
cpg	1149.45	J/mol×K	1005.78	Joback Method
cpg	1163.00	J/mol×K	1040.79	Joback Method
cpg	1175.54	J/mol×K	1075.81	Joback Method
cpg	1187.12	J/mol×K	1110.82	Joback Method
cpg	1197.81	J/mol×K	1145.84	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=U393627&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