Glutaric acid, tridec-2-yn-1-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C25H32F4O4/c1-2-3-4-5-6-7-8-9-10-11-12-19-32-22(30)17-14-18-23(31)33-21

InchiKey: MXQVHQHGTHJDIZ-UHFFFAOYSA-N

Formula: C25H32F4O4

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

Mol. weight [g/mol]: 472.51

Physical Properties

Property code	Value	Unit	Source
gf	-788.67	kJ/mol	Joback Method
hf	-1356.23	kJ/mol	Joback Method
hfus	67.37	kJ/mol	Joback Method
hvap	90.74	kJ/mol	Joback Method
log10ws	-8.58		Crippen Method
logp	6.998		Crippen Method
mcvol	352.710	ml/mol	McGowan Method
pc	960.88	kPa	Joback Method
rinpol	2817.00		NIST Webbook
rinpol	2817.00		NIST Webbook
tb	963.47	K	Joback Method
tc	1179.69	K	Joback Method
tf	678.17	K	Joback Method
vc	1.399	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1152.65	J/mol×K	963.47	Joback Method
cpg	1167.96	J/mol×K	999.51	Joback Method
cpg	1181.98	J/mol×K	1035.54	Joback Method
cpg	1194.77	J/mol×K	1071.58	Joback Method
cpg	1206.38	J/mol×K	1107.62	Joback Method
cpg	1216.88	J/mol×K	1143.65	Joback Method
cpg	1226.32	J/mol×K	1179.69	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=U393628&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