Glutaric acid, tridec-2-yn-1-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C24H31F3O4/c1-2-3-4-5-6-7-8-9-10-11-12-18-30-21(28)14-13-15-22(29)31-20

InchiKey: VXHVYYVPKLVYMQ-UHFFFAOYSA-N

Formula: C24H31F3O4

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

Mol. weight [g/mol]: 440.50

Physical Properties

Property code	Value	Unit	Source
gf	-614.75	kJ/mol	Joback Method
hf	-1142.20	kJ/mol	Joback Method
hfus	68.73	kJ/mol	Joback Method
hvap	91.29	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.257		Crippen Method
mcvol	336.850	ml/mol	McGowan Method
pc	1027.94	kPa	Joback Method
rinpol	2825.00		NIST Webbook
tb	949.53	K	Joback Method
tc	1162.50	K	Joback Method
tf	676.41	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1083.93	J/mol×K	949.53	Joback Method
cpg	1099.03	J/mol×K	985.02	Joback Method
cpg	1112.78	J/mol×K	1020.52	Joback Method
cpg	1125.22	J/mol×K	1056.01	Joback Method
cpg	1136.36	J/mol×K	1091.51	Joback Method
cpg	1146.23	J/mol×K	1127.00	Joback Method
cpg	1154.85	J/mol×K	1162.50	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393649&Units=SI
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

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