Glutaric acid, tridec-2-yn-1-yl 4-fluoro-2-methoxyphenyl ester

Inchi: InChI=1S/C25H35FO5/c1-3-4-5-6-7-8-9-10-11-12-13-19-30-24(27)15-14-16-25(28)31-22

InchiKey: ZCDKEKMPILSXKY-UHFFFAOYSA-N

Formula: C25H35FO5

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)Oc1ccc(F)cc1OC

Mol. weight [g/mol]: 434.54

Physical Properties

Property code	Value	Unit	Source
gf	-312.08	kJ/mol	Joback Method
hf	-891.37	kJ/mol	Joback Method
hfus	66.73	kJ/mol	Joback Method
hvap	96.90	kJ/mol	Joback Method
log10ws	-7.59		Crippen Method
logp	5.987		Crippen Method
mcvol	353.270	ml/mol	McGowan Method
pc	1022.69	kPa	Joback Method
rinpol	3046.00		NIST Webbook
rinpol	3046.00		NIST Webbook
tb	991.31	K	Joback Method
tc	1213.64	K	Joback Method
tf	696.21	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1160.33	J/mol×K	991.31	Joback Method
cpg	1175.29	J/mol×K	1028.37	Joback Method
cpg	1188.62	J/mol×K	1065.42	Joback Method
cpg	1200.36	J/mol×K	1102.48	Joback Method
cpg	1210.52	J/mol×K	1139.53	Joback Method
cpg	1219.12	J/mol×K	1176.59	Joback Method
cpg	1226.18	J/mol×K	1213.64	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393454&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

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