Glutaric acid, dec-2-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C22H30F4O4/c1-3-4-5-6-7-8-11-16(2)29-19(27)14-10-15-20(28)30-18-13-9-12

InchiKey: LQARVVHRGMEWHV-UHFFFAOYSA-N

Formula: C22H30F4O4

SMILES: CCCCCCCCC(C)OC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 434.46

Physical Properties

Property code	Value	Unit	Source
gf	-1019.17	kJ/mol	Joback Method
hf	-1571.89	kJ/mol	Joback Method
hfus	52.96	kJ/mol	Joback Method
hvap	81.53	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	6.603		Crippen Method
mcvol	319.040	ml/mol	McGowan Method
pc	1047.33	kPa	Joback Method
rinpol	2374.00		NIST Webbook
rinpol	2374.00		NIST Webbook
tb	885.39	K	Joback Method
tc	1084.53	K	Joback Method
tf	523.26	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1026.46	J/mol×K	885.39	Joback Method
cpg	1041.92	J/mol×K	918.58	Joback Method
cpg	1056.22	J/mol×K	951.77	Joback Method
cpg	1069.42	J/mol×K	984.96	Joback Method
cpg	1081.56	J/mol×K	1018.15	Joback Method
cpg	1092.67	J/mol×K	1051.34	Joback Method
cpg	1102.81	J/mol×K	1084.53	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=U393625&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