Glutaric acid, 1,1,1-trifluoroprop-2-yl tetradecyl ester

Inchi: InChI=1S/C22H39F3O4/c1-3-4-5-6-7-8-9-10-11-12-13-14-18-28-20(26)16-15-17-21(27)2
InchiKey: VHQVQBRBJHVFPM-UHFFFAOYSA-N
Formula: C22H39F3O4
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 424.54

Physical Properties

Property code	Value	Unit	Source
gf	-917.51	kJ/mol	Joback Method
hf	-1589.37	kJ/mol	Joback Method
hfus	56.61	kJ/mol	Joback Method
hvap	78.74	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	6.895		Crippen Method
mcvol	341.030	ml/mol	McGowan Method
pc	893.20	kPa	Joback Method
rinpol	2349.00		NIST Webbook
rinpol	2349.00		NIST Webbook
tb	849.48	K	Joback Method
tc	1040.26	K	Joback Method
tf	471.21	K	Joback Method
vc	1.353	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.77	J/mol×K	849.48	Joback Method
cpg	1133.32	J/mol×K	881.28	Joback Method
cpg	1150.71	J/mol×K	913.07	Joback Method
cpg	1166.96	J/mol×K	944.87	Joback Method
cpg	1182.13	J/mol×K	976.66	Joback Method
cpg	1196.24	J/mol×K	1008.46	Joback Method
cpg	1209.35	J/mol×K	1040.26	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=U391634&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