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

Inchi: InChI=1S/C21H37F3O4/c1-3-4-5-6-7-8-9-10-11-12-13-17-27-19(25)15-14-16-20(26)28-1
InchiKey: AMXBJUOJUWCTQW-UHFFFAOYSA-N
Formula: C21H37F3O4
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 410.51

Physical Properties

Property code	Value	Unit	Source
gf	-925.93	kJ/mol	Joback Method
hf	-1568.73	kJ/mol	Joback Method
hfus	54.02	kJ/mol	Joback Method
hvap	76.52	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.505		Crippen Method
mcvol	326.940	ml/mol	McGowan Method
pc	946.75	kPa	Joback Method
rinpol	2249.00		NIST Webbook
rinpol	2249.00		NIST Webbook
tb	826.60	K	Joback Method
tc	1012.02	K	Joback Method
tf	459.94	K	Joback Method
vc	1.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1053.49	J/mol×K	826.60	Joback Method
cpg	1071.50	J/mol×K	857.50	Joback Method
cpg	1088.42	J/mol×K	888.41	Joback Method
cpg	1104.29	J/mol×K	919.31	Joback Method
cpg	1119.13	J/mol×K	950.21	Joback Method
cpg	1132.99	J/mol×K	981.12	Joback Method
cpg	1145.91	J/mol×K	1012.02	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=U391624&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