Glutaric acid, 2,2,2-triluoroethyl hexyl ester

Inchi: InChI=1S/C13H21F3O4/c1-2-3-4-5-9-19-11(17)7-6-8-12(18)20-10-13(14,15)16/h2-10H2,
InchiKey: NWJOVVPNUBUWCU-UHFFFAOYSA-N
Formula: C13H21F3O4
SMILES: CCCCCCOC(=O)CCCC(=O)OCC(F)(F)F
Mol. weight [g/mol]: 298.30

Physical Properties

Property code	Value	Unit	Source
gf	-990.85	kJ/mol	Joback Method
hf	-1398.33	kJ/mol	Joback Method
hfus	36.83	kJ/mol	Joback Method
hvap	59.10	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.386		Crippen Method
mcvol	214.220	ml/mol	McGowan Method
pc	1612.88	kPa	Joback Method
rinpol	1532.00		NIST Webbook
rinpol	1532.00		NIST Webbook
tb	644.00	K	Joback Method
tc	810.37	K	Joback Method
tf	384.78	K	Joback Method
vc	0.855	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	595.15	J/mol×K	644.00	Joback Method
cpg	609.14	J/mol×K	671.73	Joback Method
cpg	622.47	J/mol×K	699.46	Joback Method
cpg	635.14	J/mol×K	727.19	Joback Method
cpg	647.17	J/mol×K	754.92	Joback Method
cpg	658.58	J/mol×K	782.65	Joback Method
cpg	669.36	J/mol×K	810.37	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=U380513&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