Glutaric acid, 1,1,1-trifluoroprop-2-yl 10-chlorodecyl ester

Inchi: InChI=1S/C18H30ClF3O4/c1-15(18(20,21)22)26-17(24)12-10-11-16(23)25-14-9-7-5-3-2-

InchiKey: WPKKENRNGBUKIU-UHFFFAOYSA-N

Formula: C18H30ClF3O4

SMILES: CC(OC(=O)CCCC(=O)OCCCCCCCCCCCCl)C(F)(F)F

Mol. weight [g/mol]: 402.88

Physical Properties

Property code	Value	Unit	Source
gf	-963.12	kJ/mol	Joback Method
hf	-1522.55	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	74.22	kJ/mol	Joback Method
log10ws	-6.01		Crippen Method
logp	5.554		Crippen Method
mcvol	296.910	ml/mol	McGowan Method
pc	1111.85	kPa	Joback Method
rinpol	2242.00		NIST Webbook
rinpol	2242.00		NIST Webbook
tb	795.39	K	Joback Method
tc	976.33	K	Joback Method
tf	456.05	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.39	J/mol×K	795.39	Joback Method
cpg	921.10	J/mol×K	825.55	Joback Method
cpg	935.86	J/mol×K	855.70	Joback Method
cpg	949.73	J/mol×K	885.86	Joback Method
cpg	962.71	J/mol×K	916.02	Joback Method
cpg	974.85	J/mol×K	946.17	Joback Method
cpg	986.17	J/mol×K	976.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392450&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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