Glutaric acid, 1,1,1-trifluoroprop-2-yl undec-2-enyl ester

Inchi: InChI=1S/C19H31F3O4/c1-3-4-5-6-7-8-9-10-11-15-25-17(23)13-12-14-18(24)26-16(2)19

InchiKey: KGIVMRHOPXJLCR-ZHACJKMWSA-N

Formula: C19H31F3O4

SMILES: CCCCCCCCC=CCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 380.44

Physical Properties

Property code	Value	Unit	Source
gf	-862.55	kJ/mol	Joback Method
hf	-1410.23	kJ/mol	Joback Method
hfus	49.04	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	5.501		Crippen Method
mcvol	294.460	ml/mol	McGowan Method
pc	1106.68	kPa	Joback Method
rinpol	2029.00		NIST Webbook
rinpol	2029.00		NIST Webbook
tb	785.00	K	Joback Method
tc	964.58	K	Joback Method
tf	432.32	K	Joback Method
vc	1.165	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	908.47	J/mol×K	785.00	Joback Method
cpg	924.88	J/mol×K	814.93	Joback Method
cpg	940.36	J/mol×K	844.86	Joback Method
cpg	954.95	J/mol×K	874.79	Joback Method
cpg	968.70	J/mol×K	904.72	Joback Method
cpg	981.64	J/mol×K	934.65	Joback Method
cpg	993.80	J/mol×K	964.58	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=U394010&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