Glutaric acid, 1,1,1-trifluoroprop-2-yl dodec-9-yn-1-yl ester

Inchi: InChI=1S/C20H31F3O4/c1-3-4-5-6-7-8-9-10-11-12-16-26-18(24)14-13-15-19(25)27-17(2

InchiKey: SRWZSOXNPBJYAL-UHFFFAOYSA-N

Formula: C20H31F3O4

SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OC(C)C(F)(F)F

Mol. weight [g/mol]: 392.45

Physical Properties

Property code	Value	Unit	Source
gf	-731.55	kJ/mol	Joback Method
hf	-1275.79	kJ/mol	Joback Method
hfus	54.55	kJ/mol	Joback Method
hvap	76.44	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.338		Crippen Method
mcvol	304.250	ml/mol	McGowan Method
pc	1115.57	kPa	Joback Method
rinpol	2192.00		NIST Webbook
rinpol	2192.00		NIST Webbook
tb	812.72	K	Joback Method
tc	999.04	K	Joback Method
tf	554.77	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.67	J/mol×K	812.72	Joback Method
cpg	960.10	J/mol×K	843.77	Joback Method
cpg	975.54	J/mol×K	874.83	Joback Method
cpg	990.01	J/mol×K	905.88	Joback Method
cpg	1003.55	J/mol×K	936.93	Joback Method
cpg	1016.18	J/mol×K	967.99	Joback Method
cpg	1027.93	J/mol×K	999.04	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=U393937&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