Glutaric acid, 1,1,1-trifluoroprop-2-yl non-5-yn-3-yl ester

Inchi: InChI=1S/C17H25F3O4/c1-4-6-7-8-10-14(5-2)24-16(22)12-9-11-15(21)23-13(3)17(18,19
InchiKey: SPEKVDURYGZRQL-UHFFFAOYSA-N
Formula: C17H25F3O4
SMILES: CCCC#CCC(CC)OC(=O)CCCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 350.37

Physical Properties

Property code	Value	Unit	Source
gf	-759.25	kJ/mol	Joback Method
hf	-1219.15	kJ/mol	Joback Method
hfus	43.26	kJ/mol	Joback Method
hvap	69.38	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.166		Crippen Method
mcvol	261.980	ml/mol	McGowan Method
pc	1373.78	kPa	Joback Method
rinpol	1766.00		NIST Webbook
rinpol	1766.00		NIST Webbook
tb	743.64	K	Joback Method
tc	927.18	K	Joback Method
tf	505.96	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	770.51	J/mol×K	743.64	Joback Method
cpg	785.96	J/mol×K	774.23	Joback Method
cpg	800.53	J/mol×K	804.82	Joback Method
cpg	814.24	J/mol×K	835.41	Joback Method
cpg	827.10	J/mol×K	866.00	Joback Method
cpg	839.14	J/mol×K	896.59	Joback Method
cpg	850.38	J/mol×K	927.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393948&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