Glutaric acid, hex-4-yn-3-yl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C17H17F3O4/c1-3-6-11(4-2)23-14(21)7-5-8-15(22)24-13-10-9-12(18)16(19)17

InchiKey: OILKXVQVVODLDP-UHFFFAOYSA-N

Formula: C17H17F3O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1ccc(F)c(F)c1F

Mol. weight [g/mol]: 342.31

Physical Properties

Property code	Value	Unit	Source
gf	-676.13	kJ/mol	Joback Method
hf	-1003.00	kJ/mol	Joback Method
hfus	47.07	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.525		Crippen Method
mcvol	238.220	ml/mol	McGowan Method
pc	1681.03	kPa	Joback Method
rinpol	2028.00		NIST Webbook
rinpol	2028.00		NIST Webbook
tb	788.93	K	Joback Method
tc	990.25	K	Joback Method
tf	582.52	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.70	J/mol×K	788.93	Joback Method
cpg	689.88	J/mol×K	822.48	Joback Method
cpg	702.15	J/mol×K	856.04	Joback Method
cpg	713.50	J/mol×K	889.59	Joback Method
cpg	723.93	J/mol×K	923.14	Joback Method
cpg	733.45	J/mol×K	956.70	Joback Method
cpg	742.06	J/mol×K	990.25	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=U393639&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