Glutaric acid, hex-4-yn-3-yl 2-fluoro-3-trifluoromethylphenyl ester

Inchi: InChI=1S/C18H18F4O4/c1-3-7-12(4-2)25-15(23)10-6-11-16(24)26-14-9-5-8-13(17(14)19

InchiKey: SWDBXIPYSSCTIM-UHFFFAOYSA-N

Formula: C18H18F4O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 374.33

Physical Properties

Property code	Value	Unit	Source
gf	-850.05	kJ/mol	Joback Method
hf	-1217.03	kJ/mol	Joback Method
hfus	45.72	kJ/mol	Joback Method
hvap	74.77	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.265		Crippen Method
mcvol	254.080	ml/mol	McGowan Method
pc	1542.71	kPa	Joback Method
rinpol	2037.00		NIST Webbook
rinpol	2037.00		NIST Webbook
tb	802.87	K	Joback Method
tc	1003.74	K	Joback Method
tf	584.28	K	Joback Method
vc	1.000	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	742.77	J/mol×K	802.87	Joback Method
cpg	756.05	J/mol×K	836.35	Joback Method
cpg	768.36	J/mol×K	869.83	Joback Method
cpg	779.73	J/mol×K	903.30	Joback Method
cpg	790.19	J/mol×K	936.78	Joback Method
cpg	799.77	J/mol×K	970.26	Joback Method
cpg	808.50	J/mol×K	1003.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393619&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