Glutaric acid, tridec-2-yn-1-yl 2-fluoroethyl ester

Inchi: InChI=1S/C20H33FO4/c1-2-3-4-5-6-7-8-9-10-11-12-17-24-19(22)14-13-15-20(23)25-18-1

InchiKey: QFCHFMRADNWQGM-UHFFFAOYSA-N

Formula: C20H33FO4

SMILES: CCCCCCCCCCC#CCOC(=O)CCCC(=O)OCCF

Mol. weight [g/mol]: 356.47

Physical Properties

Property code	Value	Unit	Source
gf	-342.33	kJ/mol	Joback Method
hf	-869.54	kJ/mol	Joback Method
hfus	59.33	kJ/mol	Joback Method
hvap	79.76	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.747		Crippen Method
mcvol	300.710	ml/mol	McGowan Method
pc	1164.04	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	817.85	K	Joback Method
tc	1005.74	K	Joback Method
tf	566.17	K	Joback Method
vc	1.183	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	927.21	J/mol×K	817.85	Joback Method
cpg	944.20	J/mol×K	849.17	Joback Method
cpg	960.18	J/mol×K	880.48	Joback Method
cpg	975.16	J/mol×K	911.80	Joback Method
cpg	989.16	J/mol×K	943.11	Joback Method
cpg	1002.19	J/mol×K	974.43	Joback Method
cpg	1014.28	J/mol×K	1005.74	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=U393721&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