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

Inchi: InChI=1S/C14H18F4O4/c1-3-6-10(4-2)22-12(20)8-5-7-11(19)21-9-14(17,18)13(15)16/h1
InchiKey: YKFVOYHGOPULPL-UHFFFAOYSA-N
Formula: C14H18F4O4
SMILES: CC#CC(CC)OC(=O)CCCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]: 326.28

Physical Properties

Property code	Value	Unit	Source
gf	-979.32	kJ/mol	Joback Method
hf	-1353.34	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	61.88	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	2.945		Crippen Method
mcvol	221.480	ml/mol	McGowan Method
pc	1659.19	kPa	Joback Method
rinpol	1602.00		NIST Webbook
rinpol	1602.00		NIST Webbook
tb	674.27	K	Joback Method
tc	853.00	K	Joback Method
tf	472.74	K	Joback Method
vc	0.878	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	614.15	J/mol×K	674.27	Joback Method
cpg	627.87	J/mol×K	704.06	Joback Method
cpg	640.84	J/mol×K	733.85	Joback Method
cpg	653.09	J/mol×K	763.64	Joback Method
cpg	664.63	J/mol×K	793.43	Joback Method
cpg	675.47	J/mol×K	823.22	Joback Method
cpg	685.63	J/mol×K	853.00	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=U393970&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