Succinic acid, hex-4-yn-3-yl 2,2,3,3,4,4,5,5-octafluoropentyl ester

Inchi: InChI=1S/C15H16F8O4/c1-3-5-9(4-2)27-11(25)7-6-10(24)26-8-13(18,19)15(22,23)14(20

InchiKey: LOCOSRAVXITGRH-UHFFFAOYSA-N

Formula: C15H16F8O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 412.27

Physical Properties

Property code	Value	Unit	Source
gf	-1744.46	kJ/mol	Joback Method
hf	-2175.92	kJ/mol	Joback Method
hfus	38.65	kJ/mol	Joback Method
hvap	58.25	kJ/mol	Joback Method
log10ws	-4.99		Crippen Method
logp	3.826		Crippen Method
mcvol	242.650	ml/mol	McGowan Method
pc	1378.88	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1620.00		NIST Webbook
tb	687.77	K	Joback Method
tc	858.02	K	Joback Method
tf	491.21	K	Joback Method
vc	0.985	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.46	J/mol×K	687.77	Joback Method
cpg	717.40	J/mol×K	716.14	Joback Method
cpg	729.54	J/mol×K	744.52	Joback Method
cpg	740.92	J/mol×K	772.89	Joback Method
cpg	751.57	J/mol×K	801.27	Joback Method
cpg	761.54	J/mol×K	829.64	Joback Method
cpg	770.87	J/mol×K	858.02	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=U390703&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