Succinic acid, hex-4-yn-3-yl pentafluorophenyl ester

Inchi: InChI=1S/C16H13F5O4/c1-3-5-8(4-2)24-9(22)6-7-10(23)25-16-14(20)12(18)11(17)13(19

InchiKey: APQQVLPUJDOCFA-UHFFFAOYSA-N

Formula: C16H13F5O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 364.26

Physical Properties

Property code	Value	Unit	Source
gf	-1093.43	kJ/mol	Joback Method
hf	-1397.52	kJ/mol	Joback Method
hfus	49.86	kJ/mol	Joback Method
hvap	72.79	kJ/mol	Joback Method
log10ws	-5.56		Crippen Method
logp	3.413		Crippen Method
mcvol	227.670	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
rinpol	1798.00		NIST Webbook
rinpol	1798.00		NIST Webbook
tb	774.55	K	Joback Method
tc	967.15	K	Joback Method
tf	597.47	K	Joback Method
vc	0.917	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.91	J/mol×K	774.55	Joback Method
cpg	646.67	J/mol×K	806.65	Joback Method
cpg	657.66	J/mol×K	838.75	Joback Method
cpg	667.87	J/mol×K	870.85	Joback Method
cpg	677.28	J/mol×K	902.95	Joback Method
cpg	685.90	J/mol×K	935.05	Joback Method
cpg	693.71	J/mol×K	967.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390349&Units=SI

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