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

Inchi: InChI=1S/C17H15F5O4/c1-3-5-9(4-2)26-12(24)7-6-11(23)25-8-10-13(18)15(20)17(22)16

InchiKey: GOLSNLJHZWDIBP-UHFFFAOYSA-N

Formula: C17H15F5O4

SMILES: CC#CC(CC)OC(=O)CCC(=O)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 378.29

Physical Properties

Property code	Value	Unit	Source
gf	-1085.01	kJ/mol	Joback Method
hf	-1418.16	kJ/mol	Joback Method
hfus	52.45	kJ/mol	Joback Method
hvap	75.01	kJ/mol	Joback Method
log10ws	-5.83		Crippen Method
logp	3.551		Crippen Method
mcvol	241.760	ml/mol	McGowan Method
pc	1527.07	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	797.43	K	Joback Method
tc	990.26	K	Joback Method
tf	608.74	K	Joback Method
vc	0.974	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	689.66	J/mol×K	797.43	Joback Method
cpg	701.85	J/mol×K	829.57	Joback Method
cpg	713.21	J/mol×K	861.71	Joback Method
cpg	723.73	J/mol×K	893.85	Joback Method
cpg	733.41	J/mol×K	925.98	Joback Method
cpg	742.24	J/mol×K	958.12	Joback Method
cpg	750.21	J/mol×K	990.26	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=U389883&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