Succinic acid, 1,1,1-trifluoroprop-2-yl non-5-yn-3-yl ester

Inchi: InChI=1S/C16H23F3O4/c1-4-6-7-8-9-13(5-2)23-15(21)11-10-14(20)22-12(3)16(17,18)19
InchiKey: NXANDDZCZMDUSW-UHFFFAOYSA-N
Formula: C16H23F3O4
SMILES: CCCC#CCC(CC)OC(=O)CCC(=O)OC(C)C(F)(F)F
Mol. weight [g/mol]: 336.35

Physical Properties

Property code	Value	Unit	Source
gf	-767.67	kJ/mol	Joback Method
hf	-1198.51	kJ/mol	Joback Method
hfus	40.67	kJ/mol	Joback Method
hvap	67.15	kJ/mol	Joback Method
log10ws	-4.93		Crippen Method
logp	3.776		Crippen Method
mcvol	247.890	ml/mol	McGowan Method
pc	1477.02	kPa	Joback Method
rinpol	1698.00		NIST Webbook
rinpol	1698.00		NIST Webbook
tb	720.76	K	Joback Method
tc	904.23	K	Joback Method
tf	494.69	K	Joback Method
vc	0.973	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	714.59	J/mol×K	720.76	Joback Method
cpg	729.68	J/mol×K	751.34	Joback Method
cpg	743.91	J/mol×K	781.92	Joback Method
cpg	757.30	J/mol×K	812.50	Joback Method
cpg	769.89	J/mol×K	843.08	Joback Method
cpg	781.68	J/mol×K	873.66	Joback Method
cpg	792.71	J/mol×K	904.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391005&Units=SI
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

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