Succinic acid, 1,1,1-trifluoroprop-2-yl 2-methyloct-5-yn-4-yl ester

Inchi: InChI=1S/C16H23F3O4/c1-5-6-7-13(10-11(2)3)23-15(21)9-8-14(20)22-12(4)16(17,18)19

InchiKey: XVUHNTLXOSBZKB-UHFFFAOYSA-N

Formula: C16H23F3O4

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

Mol. weight [g/mol]: 336.35

Physical Properties

Property code	Value	Unit	Source
gf	-770.11	kJ/mol	Joback Method
hf	-1203.79	kJ/mol	Joback Method
hfus	37.15	kJ/mol	Joback Method
hvap	66.76	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	3.632		Crippen Method
mcvol	247.890	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinpol	1637.00		NIST Webbook
rinpol	1637.00		NIST Webbook
tb	720.32	K	Joback Method
tc	906.07	K	Joback Method
tf	479.69	K	Joback Method
vc	0.967	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	715.10	J/mol×K	720.32	Joback Method
cpg	730.39	J/mol×K	751.28	Joback Method
cpg	744.80	J/mol×K	782.24	Joback Method
cpg	758.35	J/mol×K	813.20	Joback Method
cpg	771.05	J/mol×K	844.16	Joback Method
cpg	782.94	J/mol×K	875.11	Joback Method
cpg	794.03	J/mol×K	906.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391022&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

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

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