

Succinic acid, 2,2,3,3-tetrafluoropropyl non-5-yn-3-yl ester

Inchi:	InChI=1S/C16H22F4O4/c1-3-5-6-7-8-12(4-2)24-14(22)10-9-13(21)23-11-16(19,20)15(17)
InchiKey:	SSQLOHJDWMEGBZ-UHFFFAOYSA-N
Formula:	C16H22F4O4
SMILES:	CCCC#CCC(CC)OC(=O)CCC(=O)OCC(F)(F)C(F)F
Mol. weight [g/mol]:	354.34

Physical Properties

Property code	Value	Unit	Source
gf	-962.48	kJ/mol	Joback Method
hf	-1394.62	kJ/mol	Joback Method
hfus	43.75	kJ/mol	Joback Method
hvap	66.33	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	3.726		Crippen Method
mvol	249.660	ml/mol	McGowan Method
pc	1427.22	kPa	Joback Method
rinpol	1781.00		NIST Webbook
rinpol	1781.00		NIST Webbook
tb	720.03	K	Joback Method
tc	898.57	K	Joback Method
tf	495.28	K	Joback Method
vc	0.991	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.38	J/molxK	720.03	Joback Method
cpg	736.99	J/molxK	749.79	Joback Method
cpg	750.79	J/molxK	779.54	Joback Method
cpg	763.79	J/molxK	809.30	Joback Method
cpg	776.02	J/molxK	839.06	Joback Method
cpg	787.49	J/molxK	868.81	Joback Method
cpg	798.22	J/molxK	898.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391006&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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