

Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl geranyl ester

Inchi:	InChI=1S/C19H24F8O4/c1-12(2)5-4-6-13(3)9-10-30-14(28)7-8-15(29)31-11-17(22,23)19
InchiKey:	CPXDHJXBIGOBPU-UKTHLTGXSA-N
Formula:	C19H24F8O4
SMILES:	CC(C)=CCCC(C)=CCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F
Mol. weight [g/mol]:	468.38

Physical Properties

Property code	Value	Unit	Source
hfus	47.20	kJ/mol	Joback Method
logp	5.717		Crippen Method
mcvol	299.010	ml/mol	McGowan Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	923.73	J/mol×K	778.81	Joback Method
cpg	938.18	J/mol×K	808.28	Joback Method
cpg	951.77	J/mol×K	837.75	Joback Method
cpg	964.58	J/mol×K	867.21	Joback Method
cpg	976.67	J/mol×K	896.68	Joback Method
cpg	988.12	J/mol×K	926.15	Joback Method
cpg	998.98	J/mol×K	955.62	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U391209&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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