

Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl oct-1-en-3-yl ester

Inchi:	InChI=1S/C17H22F8O4/c1-3-5-6-7-11(4-2)29-13(27)9-8-12(26)28-10-15(20,21)17(24,25)
InchiKey:	JIVBAFYRBXRTRY-UHFFFAOYSA-N
Formula:	C17H22F8O4
SMILES:	<chem>C=CC(CCCCC)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F</chem>
Mol. weight [g/mol]:	442.34

Physical Properties

Property code	Value	Unit	Source
gf	-1842.58	kJ/mol	Joback Method
hf	-2364.07	kJ/mol	Joback Method
hfus	39.43	kJ/mol	Joback Method
hvap	59.88	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	5.159		Crippen Method
mvol	275.130	ml/mol	McGowan Method
pc	1108.89	kPa	Joback Method
rinpol	1754.00		NIST Webbook
rinpol	1754.00		NIST Webbook
tb	721.21	K	Joback Method
tc	886.95	K	Joback Method
tf	405.89	K	Joback Method
vc	1.115	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	834.80	J/mol×K	721.21	Joback Method
cpg	849.02	J/mol×K	748.83	Joback Method
cpg	862.40	J/mol×K	776.46	Joback Method
cpg	874.98	J/mol×K	804.08	Joback Method
cpg	886.80	J/mol×K	831.70	Joback Method
cpg	897.90	J/mol×K	859.33	Joback Method
cpg	908.34	J/mol×K	886.95	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391316&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
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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