

Succinic acid, dodec-2-en-1-yl 2,2,3,3,3-pentafluoropropyl ester

Inchi:	InChI=1S/C19H29F5O4/c1-2-3-4-5-6-7-8-9-10-11-14-27-16(25)12-13-17(26)28-15-18(20)
InchiKey:	CGFFMQLHRFUWQT-ZHACJKMWSA-N
Formula:	C19H29F5O4
SMILES:	CCCCCCCCC=CCOC(=O)CCC(=O)OCC(F)(F)C(F)(F)F
Mol. weight [g/mol]:	416.42

Physical Properties

Property code	Value	Unit	Source
gf	-1246.89	kJ/mol	Joback Method
hf	-1805.92	kJ/mol	Joback Method
hfus	51.31	kJ/mol	Joback Method
hvap	69.48	kJ/mol	Joback Method
log10ws	-6.33		Crippen Method
logp	5.747		Crippen Method
mvol	298.000	ml/mol	McGowan Method
pc	1050.73	kPa	Joback Method
rinpol	2010.00		NIST Webbook
rinpol	2010.00		NIST Webbook
tb	780.75	K	Joback Method
tc	957.49	K	Joback Method
tf	450.92	K	Joback Method
vc	1.196	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	924.50	J/mol×K	780.75	Joback Method
cpg	940.24	J/mol×K	810.21	Joback Method
cpg	955.10	J/mol×K	839.66	Joback Method
cpg	969.10	J/mol×K	869.12	Joback Method
cpg	982.30	J/mol×K	898.58	Joback Method
cpg	994.75	J/mol×K	928.03	Joback Method
cpg	1006.50	J/mol×K	957.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390876&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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