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

Inchi: InChI=1S/C16H22F8O4/c1-3-4-5-6-10(2)28-12(26)8-7-11(25)27-9-14(19,20)16(23,24)15(

InchiKey: MJSQKRGPEQAEEC-UHFFFAOYSA-N

Formula: C16H22F8O4

SMILES: CCCCCC(C)OC(=O)CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F

Mol. weight [g/mol]: 430.33

Physical Properties

Property code	Value	Unit	Source
gf	-1938.84	kJ/mol	Joback Method
hf	-2468.86	kJ/mol	Joback Method
hfus	38.12	kJ/mol	Joback Method
hvap	58.32	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.993		Crippen Method
mcvol	265.340	ml/mol	McGowan Method
pc	1149.87	kPa	Joback Method
rinpol	1654.00		NIST Webbook
rinpol	1654.00		NIST Webbook
tb	701.65	K	Joback Method
tc	864.31	K	Joback Method
tf	396.38	K	Joback Method
vc	1.079	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	803.42	J/mol×K	701.65	Joback Method
cpg	817.74	J/mol×K	728.76	Joback Method
cpg	831.24	J/mol×K	755.87	Joback Method
cpg	843.95	J/mol×K	782.98	Joback Method
cpg	855.92	J/mol×K	810.09	Joback Method
cpg	867.17	J/mol×K	837.20	Joback Method
cpg	877.75	J/mol×K	864.31	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390566&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
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

Latest version available from:
https://www.chemeo.com/cid/115-946-4/Succinic-acid-2-2-3-3-4-4-5-5-octafluoropentyl-2-heptyl-ester.pdf
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