

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

Inchi:	InChI=1S/C16H9F13O4/c17-8-5(9(18)11(20)12(21)10(8)19)3-32-6(30)1-2-7(31)33-4-14(2
InchiKey:	NITFPYAZMCLHLU-UHFFFAOYSA-N
Formula:	C16H9F13O4
SMILES:	O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	512.22

Physical Properties

Property code	Value	Unit	Source
gf	-2846.19	kJ/mol	Joback Method
hf	-3264.95	kJ/mol	Joback Method
hfus	49.14	kJ/mol	Joback Method
hvap	60.21	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	4.920		Crippen Method
mcvol	250.430	ml/mol	McGowan Method
pc	1168.02	kPa	Joback Method
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook
tb	750.02	K	Joback Method
tc	919.30	K	Joback Method
tf	503.35	K	Joback Method
vc	1.067	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	752.55	J/molxK	750.02	Joback Method
cpg	763.04	J/molxK	778.23	Joback Method
cpg	772.81	J/molxK	806.45	Joback Method
cpg	781.89	J/molxK	834.66	Joback Method
cpg	790.31	J/molxK	862.87	Joback Method
cpg	798.11	J/molxK	891.08	Joback Method
cpg	805.32	J/molxK	919.30	Joback Method

Sources

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=U389878&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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