

Succinic acid, 2-ethylhexyl pentafluorophenyl ester

Inchi:	InChI=1S/C18H21F5O4/c1-3-5-6-10(4-2)9-26-11(24)7-8-12(25)27-18-16(22)14(20)13(19)
InchiKey:	ORIUBXVWUROFRX-UHFFFAOYSA-N
Formula:	C18H21F5O4
SMILES:	CCCCC(CC)COC(=O)CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	396.35

Physical Properties

Property code	Value	Unit	Source
gf	-1279.39	kJ/mol	Joback Method
hf	-1711.10	kJ/mol	Joback Method
hfus	51.92	kJ/mol	Joback Method
hvap	75.09	kJ/mol	Joback Method
log10ws	-6.25		Crippen Method
logp	4.827		Crippen Method
mcvol	264.450	ml/mol	McGowan Method
pc	1261.95	kPa	Joback Method
rinpol	1940.00		NIST Webbook
rinpol	1940.00		NIST Webbook
tb	811.31	K	Joback Method
tc	996.92	K	Joback Method
tf	513.91	K	Joback Method
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	796.29	J/mol×K	811.31	Joback Method
cpg	809.86	J/mol×K	842.25	Joback Method
cpg	822.54	J/mol×K	873.18	Joback Method
cpg	834.32	J/mol×K	904.12	Joback Method
cpg	845.21	J/mol×K	935.05	Joback Method
cpg	855.21	J/mol×K	965.99	Joback Method
cpg	864.31	J/mol×K	996.92	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=U390351&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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