

Succinic acid, di(pentafluorophenyl) ester

Inchi: InChI=1S/C16H4F10O4/c17-5-7(19)11(23)15(12(24)8(5)20)29-3(27)1-2-4(28)30-16-13(2)
InchiKey: OQCVCUZWJWLXHG-UHFFFAOYSA-N
Formula: C16H4F10O4
SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)Oc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 450.18

Physical Properties

Property code	Value	Unit	Source
gf	-2203.58	kJ/mol	Joback Method
hf	-2465.91	kJ/mol	Joback Method
hfus	57.76	kJ/mol	Joback Method
hvap	72.52	kJ/mol	Joback Method
log10ws	-7.06		Crippen Method
logp	4.369		Crippen Method
mvol	221.360	ml/mol	McGowan Method
pc	1479.29	kPa	Joback Method
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook
tb	813.92	K	Joback Method
tc	999.84	K	Joback Method
tf	598.34	K	Joback Method
vc	0.944	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	621.62	J/mol×K	813.92	Joback Method
cpg	630.36	J/mol×K	844.91	Joback Method
cpg	638.40	J/mol×K	875.89	Joback Method
cpg	645.70	J/mol×K	906.88	Joback Method
cpg	652.25	J/mol×K	937.87	Joback Method
cpg	658.04	J/mol×K	968.85	Joback Method
cpg	663.05	J/mol×K	999.84	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U390359&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

Latest version available from:

<https://www.chemeo.com/cid/122-383-1/Succinic-acid-di-pentafluorophenyl-ester.pdf>

Generated by Cheméo on 2024-04-28 13:47:52.668751353 +0000 UTC m=+16601321.589328668.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.