

Succinic acid, isobutyl 1-(pentafluorophenyl)ethyl ester

Inchi:	InChI=1S/C16H17F5O4/c1-7(2)6-24-9(22)4-5-10(23)25-8(3)11-12(17)14(19)16(21)15(20)
InchiKey:	SSQKRUANSQNICG-UHFFFAOYSA-N
Formula:	C16H17F5O4
SMILES:	CC(C)COC(=O)CCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]:	368.30

Physical Properties

Property code	Value	Unit	Source
gf	-1298.67	kJ/mol	Joback Method
hf	-1675.10	kJ/mol	Joback Method
hfus	43.22	kJ/mol	Joback Method
hvap	70.25	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	3.966		Crippen Method
mcvol	236.270	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	1772.00		NIST Webbook
rinpol	1772.00		NIST Webbook
tb	765.11	K	Joback Method
tc	948.27	K	Joback Method
tf	476.37	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.58	J/molxK	765.11	Joback Method
cpg	697.36	J/molxK	795.64	Joback Method
cpg	709.35	J/molxK	826.16	Joback Method
cpg	720.55	J/molxK	856.69	Joback Method
cpg	730.97	J/molxK	887.22	Joback Method
cpg	740.59	J/molxK	917.75	Joback Method
cpg	749.41	J/molxK	948.27	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U380822&Units=SI
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

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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