

Succinic acid, 4-isopropylphenyl pentafluorobenzyl ester

Inchi:	InChI=1S/C20H17F5O4/c1-10(2)11-3-5-12(6-4-11)29-15(27)8-7-14(26)28-9-13-16(21)18
InchiKey:	KUGCDOLBKKHYDL-UHFFFAOYSA-N
Formula:	C20H17F5O4
SMILES:	CC(C)c1ccc(OC(=O)CCC(=O)OCc2c(F)c(F)c(F)c(F)c2F)cc1
Mol. weight [g/mol]:	416.34

Physical Properties

Property code	Value	Unit	Source
gf	-1159.77	kJ/mol	Joback Method
hf	-1527.32	kJ/mol	Joback Method
hfus	50.76	kJ/mol	Joback Method
hvap	82.48	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	4.934		Crippen Method
mvol	268.870	ml/mol	McGowan Method
pc	1380.93	kPa	Joback Method
rinpol	2398.00		NIST Webbook
rinpol	2398.00		NIST Webbook
tb	888.73	K	Joback Method
tc	1094.42	K	Joback Method
tf	575.39	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	812.51	J/mol×K	888.73	Joback Method
cpg	824.31	J/mol×K	923.01	Joback Method
cpg	835.00	J/mol×K	957.29	Joback Method
cpg	844.59	J/mol×K	991.57	Joback Method
cpg	853.09	J/mol×K	1025.85	Joback Method
cpg	860.49	J/mol×K	1060.13	Joback Method
cpg	866.82	J/mol×K	1094.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360720&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
h vap:	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
r in pol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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