Succinic acid, cyclohexylmethyl pentafluorophenyl ester

Inchi: InChI=1S/C17H17F5O4/c18-12-13(19)15(21)17(16(22)14(12)20)26-11(24)7-6-10(23)25-8

InchiKey: QXDJOKYPWIJHQS-UHFFFAOYSA-N

Formula: C17H17F5O4

SMILES: O=C(CCC(=O)Oc1c(F)c(F)c(F)c(F)c1F)OCC1CCCCC1

Mol. weight [g/mol]: 380.31

Physical Properties

Property code	Value	Unit	Source
gf	-1260.92	kJ/mol	Joback Method
hf	-1630.86	kJ/mol	Joback Method
hfus	44.69	kJ/mol	Joback Method
hvap	73.68	kJ/mol	Joback Method
log10ws	-5.73		Crippen Method
logp	4.191		Crippen Method
mcvol	239.500	ml/mol	McGowan Method
pc	1572.21	kPa	Joback Method
rinpol	2006.00		NIST Webbook
rinpol	2006.00		NIST Webbook
tb	808.42	K	Joback Method
tc	1005.37	K	Joback Method
tf	525.02	K	Joback Method
vc	0.951	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.83	J/mol×K	808.42	Joback Method
cpg	746.59	J/mol×K	841.24	Joback Method
cpg	759.29	J/mol×K	874.07	Joback Method
cpg	770.92	J/mol×K	906.89	Joback Method
cpg	781.49	J/mol×K	939.72	Joback Method
cpg	790.99	J/mol×K	972.54	Joback Method
cpg	799.42	J/mol×K	1005.37	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390352&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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