Succinic acid, cyclohexylmethyl pentafluorobenzyl ester

Inchi: InChI=1S/C18H19F5O4/c19-14-11(15(20)17(22)18(23)16(14)21)9-27-13(25)7-6-12(24)2

InchiKey: ZHMZQTHUPDJPEM-UHFFFAOYSA-N

Formula: C18H19F5O4

SMILES: O=C(CCC(=O)OCC1CCCCC1)OCc1c(F)c(F)c(F)c(F)c1F

Mol. weight [g/mol]: 394.33

Physical Properties

Property code	Value	Unit	Source
gf	-1252.50	kJ/mol	Joback Method
hf	-1651.50	kJ/mol	Joback Method
hfus	47.28	kJ/mol	Joback Method
hvap	75.90	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	4.329		Crippen Method
mcvol	253.590	ml/mol	McGowan Method
pc	1459.02	kPa	Joback Method
rinpol	2215.00		NIST Webbook
rinpol	2215.00		NIST Webbook
tb	831.30	K	Joback Method
tc	1028.83	K	Joback Method
tf	536.29	K	Joback Method
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	789.84	J/mol×K	831.30	Joback Method
cpg	803.84	J/mol×K	864.22	Joback Method
cpg	816.71	J/mol×K	897.14	Joback Method
cpg	828.46	J/mol×K	930.06	Joback Method
cpg	839.09	J/mol×K	962.98	Joback Method
cpg	848.60	J/mol×K	995.91	Joback Method
cpg	857.00	J/mol×K	1028.83	Joback Method

Sources

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=U389886&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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