Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C22H18F8O5/c23-19(24)21(27,28)22(29,30)20(25,26)13-34-18(32)10-9-17(31)

InchiKey: VIXUWGTXQDJDHA-UHFFFAOYSA-N

Formula: C22H18F8O5

SMILES: O=C(CCC(=O)OCC(F)(F)C(F)(F)C(F)(F)C(F)F)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 514.36

Physical Properties

Property code	Value	Unit	Source
gf	-1775.69	kJ/mol	Joback Method
hf	-2258.05	kJ/mol	Joback Method
hfus	46.07	kJ/mol	Joback Method
hvap	79.69	kJ/mol	Joback Method
log10ws	-6.73		Crippen Method
logp	6.016		Crippen Method
mcvol	308.230	ml/mol	McGowan Method
pc	1186.60	kPa	Joback Method
rinpol	2488.00		NIST Webbook
rinpol	2488.00		NIST Webbook
tb	920.13	K	Joback Method
tc	1128.55	K	Joback Method
tf	566.59	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	984.62	J/mol×K	920.13	Joback Method
cpg	996.02	J/mol×K	954.87	Joback Method
cpg	1006.37	J/mol×K	989.60	Joback Method
cpg	1015.77	J/mol×K	1024.34	Joback Method
cpg	1024.30	J/mol×K	1059.07	Joback Method
cpg	1032.05	J/mol×K	1093.81	Joback Method
cpg	1039.12	J/mol×K	1128.55	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=U390363&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