Succinic acid, 2,2,3,3-tetrafluoropropyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C20H18F4O5/c21-19(22)20(23,24)13-28-18(26)10-9-17(25)27-12-14-5-4-8-16(

InchiKey: FBFNWUUHMVTLOC-UHFFFAOYSA-N

Formula: C20H18F4O5

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

Mol. weight [g/mol]: 414.35

Physical Properties

Property code	Value	Unit	Source
gf	-1018.97	kJ/mol	Joback Method
hf	-1414.83	kJ/mol	Joback Method
hfus	43.39	kJ/mol	Joback Method
hvap	81.10	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	4.746		Crippen Method
mcvol	272.970	ml/mol	McGowan Method
pc	1515.21	kPa	Joback Method
rinpol	2425.00		NIST Webbook
rinpol	2425.00		NIST Webbook
tb	883.75	K	Joback Method
tc	1094.38	K	Joback Method
tf	536.85	K	Joback Method
vc	1.060	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.31	J/mol×K	883.75	Joback Method
cpg	851.39	J/mol×K	918.86	Joback Method
cpg	862.30	J/mol×K	953.96	Joback Method
cpg	872.07	J/mol×K	989.07	Joback Method
cpg	880.75	J/mol×K	1024.17	Joback Method
cpg	888.38	J/mol×K	1059.28	Joback Method
cpg	895.00	J/mol×K	1094.38	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390362&Units=SI

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