Succinic acid, 1,1,1-trifluoroprop-2-yl 3-phenoxybenzyl ester

Inchi: InChI=1S/C20H19F3O5/c1-14(20(21,22)23)27-19(25)11-10-18(24)26-13-15-6-5-9-17(12-

InchiKey: WKPFESIEVIVMMO-UHFFFAOYSA-N

Formula: C20H19F3O5

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

Mol. weight [g/mol]: 396.36

Physical Properties

Property code	Value	Unit	Source
gf	-824.16	kJ/mol	Joback Method
hf	-1218.72	kJ/mol	Joback Method
hfus	40.31	kJ/mol	Joback Method
hvap	81.92	kJ/mol	Joback Method
log10ws	-5.42		Crippen Method
logp	4.796		Crippen Method
mcvol	271.200	ml/mol	McGowan Method
pc	1569.72	kPa	Joback Method
rinpol	2329.00		NIST Webbook
rinpol	2329.00		NIST Webbook
tb	884.48	K	Joback Method
tc	1099.80	K	Joback Method
tf	536.26	K	Joback Method
vc	1.042	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	832.02	J/mol×K	884.48	Joback Method
cpg	844.48	J/mol×K	920.37	Joback Method
cpg	855.71	J/mol×K	956.25	Joback Method
cpg	865.76	J/mol×K	992.14	Joback Method
cpg	874.68	J/mol×K	1028.03	Joback Method
cpg	882.50	J/mol×K	1063.92	Joback Method
cpg	889.28	J/mol×K	1099.80	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390361&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

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