Succinic acid, 2-fluorophenyl 3-phenoxybenzyl ester

Inchi: InChI=1S/C23H19FO5/c24-20-11-4-5-12-21(20)29-23(26)14-13-22(25)27-16-17-7-6-10-1

InchiKey: HHJUWODPRZWAEE-UHFFFAOYSA-N

Formula: C23H19FO5

SMILES: O=C(CCC(=O)Oc1ccccc1F)OCc1cccc(Oc2ccccc2)c1

Mol. weight [g/mol]: 394.39

Physical Properties

Property code	Value	Unit	Source
gf	-306.90	kJ/mol	Joback Method
hf	-649.33	kJ/mol	Joback Method
hfus	46.51	kJ/mol	Joback Method
hvap	94.85	kJ/mol	Joback Method
log10ws	-5.98		Crippen Method
logp	5.047		Crippen Method
mcvol	286.170	ml/mol	McGowan Method
pc	1689.34	kPa	Joback Method
rinpol	2979.00		NIST Webbook
rinpol	2979.00		NIST Webbook
tb	989.91	K	Joback Method
tc	1230.22	K	Joback Method
tf	620.41	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	882.09	J/mol×K	989.91	Joback Method
cpg	892.53	J/mol×K	1029.96	Joback Method
cpg	901.41	J/mol×K	1070.01	Joback Method
cpg	908.78	J/mol×K	1110.06	Joback Method
cpg	914.67	J/mol×K	1150.12	Joback Method
cpg	919.13	J/mol×K	1190.17	Joback Method
cpg	922.21	J/mol×K	1230.22	Joback Method

Sources

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=U390371&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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