

Succinic acid, 2-fluorophenyl 4-biphenyl ester

Inchi: InChI=1S/C22H17FO4/c23-19-8-4-5-9-20(19)27-22(25)15-14-21(24)26-18-12-10-17(11-12)
InchiKey: ZORJSRRIXHMJFC-UHFFFAOYSA-N
Formula: C22H17FO4
SMILES: O=C(CCC(=O)Oc1ccccc1F)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 364.37

Physical Properties

Property code	Value	Unit	Source
gf	-210.32	kJ/mol	Joback Method
hf	-496.47	kJ/mol	Joback Method
hfus	42.73	kJ/mol	Joback Method
hvap	90.21	kJ/mol	Joback Method
log10ws	-6.68		Crippen Method
logp	4.784		Crippen Method
mvol	266.210	ml/mol	McGowan Method
pc	1857.91	kPa	Joback Method
rinpol	3089.00		NIST Webbook
rinpol	3089.00		NIST Webbook
tb	944.61	K	Joback Method
tc	1187.41	K	Joback Method
tf	586.91	K	Joback Method
vc	1.010	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.38	J/molxK	944.61	Joback Method
cpg	810.89	J/molxK	985.08	Joback Method
cpg	821.00	J/molxK	1025.54	Joback Method
cpg	829.75	J/molxK	1066.01	Joback Method
cpg	837.22	J/molxK	1106.48	Joback Method
cpg	843.46	J/molxK	1146.95	Joback Method
cpg	848.54	J/molxK	1187.41	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=U390086&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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