Succinic acid, naphth-2-ylmethyl 3-fluorophenyl ester

Inchi: InChI=1S/C21H17FO4/c22-18-6-3-7-19(13-18)26-21(24)11-10-20(23)25-14-15-8-9-16-4-

InchiKey: ZHOGLMNGLYNHEI-UHFFFAOYSA-N

Formula: C21H17FO4

SMILES: O=C(CCC(=O)Oc1cccc(F)c1)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 352.36

Physical Properties

Property code	Value	Unit	Source
gf	-224.50	kJ/mol	Joback Method
hf	-521.29	kJ/mol	Joback Method
hfus	43.12	kJ/mol	Joback Method
hvap	87.35	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	4.408		Crippen Method
mcvol	256.420	ml/mol	McGowan Method
pc	1874.03	kPa	Joback Method
rinpol	2849.00		NIST Webbook
rinpol	2849.00		NIST Webbook
tb	914.03	K	Joback Method
tc	1147.93	K	Joback Method
tf	581.92	K	Joback Method
vc	0.984	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.64	J/mol×K	914.03	Joback Method
cpg	777.79	J/mol×K	953.01	Joback Method
cpg	788.80	J/mol×K	992.00	Joback Method
cpg	798.76	J/mol×K	1030.98	Joback Method
cpg	807.73	J/mol×K	1069.96	Joback Method
cpg	815.78	J/mol×K	1108.95	Joback Method
cpg	822.98	J/mol×K	1147.93	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=U390342&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