Succinic acid, 2-naphthylmethyl 2-fluoro-3-(trifluoromethyl)phenyl ester

Inchi: InChI=1S/C22H16F4O4/c23-21-17(22(24,25)26)6-3-7-18(21)30-20(28)11-10-19(27)29-13

InchiKey: ZKZBOIGZEHGIEO-UHFFFAOYSA-N

Formula: C22H16F4O4

SMILES: O=C(CCC(=O)Oc1cccc(C(F)(F)F)c1F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 420.35

Physical Properties

Property code	Value	Unit	Source
gf	-807.30	kJ/mol	Joback Method
hf	-1150.48	kJ/mol	Joback Method
hfus	47.15	kJ/mol	Joback Method
hvap	86.49	kJ/mol	Joback Method
log10ws	-7.25		Crippen Method
logp	5.427		Crippen Method
mcvol	275.820	ml/mol	McGowan Method
pc	1553.67	kPa	Joback Method
rinpol	2928.00		NIST Webbook
rinpol	2928.00		NIST Webbook
tb	936.47	K	Joback Method
tc	1159.95	K	Joback Method
tf	609.90	K	Joback Method
vc	1.083	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.61	J/mol×K	936.47	Joback Method
cpg	854.83	J/mol×K	973.72	Joback Method
cpg	865.09	J/mol×K	1010.96	Joback Method
cpg	874.47	J/mol×K	1048.21	Joback Method
cpg	883.05	J/mol×K	1085.45	Joback Method
cpg	890.94	J/mol×K	1122.70	Joback Method
cpg	898.20	J/mol×K	1159.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390795&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