Succinic acid, naphth-2-ylmethyl 2,3,4-trifluorophenyl ester

Inchi: InChI=1S/C21H15F3O4/c22-16-7-8-17(21(24)20(16)23)28-19(26)10-9-18(25)27-12-13-5-

InchiKey: STQSZZHFAFRZPK-UHFFFAOYSA-N

Formula: C21H15F3O4

SMILES: O=C(CCC(=O)Oc1ccc(F)c(F)c1F)OCc1ccc2ccccc2c1

Mol. weight [g/mol]: 388.34

Physical Properties

Property code	Value	Unit	Source
gf	-633.38	kJ/mol	Joback Method
hf	-936.45	kJ/mol	Joback Method
hfus	48.50	kJ/mol	Joback Method
hvap	87.04	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	4.686		Crippen Method
mcvol	259.960	ml/mol	McGowan Method
pc	1693.51	kPa	Joback Method
rinpol	2894.00		NIST Webbook
rinpol	2894.00		NIST Webbook
tb	922.53	K	Joback Method
tc	1146.11	K	Joback Method
tf	608.14	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	777.05	J/mol×K	922.53	Joback Method
cpg	788.17	J/mol×K	959.79	Joback Method
cpg	798.24	J/mol×K	997.06	Joback Method
cpg	807.31	J/mol×K	1034.32	Joback Method
cpg	815.44	J/mol×K	1071.58	Joback Method
cpg	822.66	J/mol×K	1108.84	Joback Method
cpg	829.03	J/mol×K	1146.11	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U390773&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