Succinic acid, 2,2,3,3-tetrafluoropropyl 4-cyanophenyl ester

Inchi: InChI=1S/C14H11F4NO4/c15-13(16)14(17,18)8-22-11(20)5-6-12(21)23-10-3-1-9(7-19)2-

InchiKey: PEHFOTYUWMATHU-UHFFFAOYSA-N

Formula: C14H11F4NO4

SMILES: N#Cc1ccc(OC(=O)CCC(=O)OCC(F)(F)C(F)F)cc1

Mol. weight [g/mol]: 333.24

Physical Properties

Property code	Value	Unit	Source
gf	-943.72	kJ/mol	Joback Method
hf	-1230.42	kJ/mol	Joback Method
hfus	34.13	kJ/mol	Joback Method
hvap	73.53	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	2.687		Crippen Method
mcvol	207.700	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	2019.00		NIST Webbook
rinpol	2019.00		NIST Webbook
tb	799.45	K	Joback Method
tc	1002.01	K	Joback Method
tf	485.57	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	594.59	J/mol×K	799.45	Joback Method
cpg	604.50	J/mol×K	833.21	Joback Method
cpg	613.58	J/mol×K	866.97	Joback Method
cpg	621.87	J/mol×K	900.73	Joback Method
cpg	629.38	J/mol×K	934.49	Joback Method
cpg	636.14	J/mol×K	968.25	Joback Method
cpg	642.18	J/mol×K	1002.01	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=U389808&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