Succinic acid, 1,1,1-trifluoroprop-2-yl 4-cyanophenyl ester

Inchi: InChI=1S/C14H12F3NO4/c1-9(14(15,16)17)21-12(19)6-7-13(20)22-11-4-2-10(8-18)3-5-1

InchiKey: KDBJGXDZRMNORF-UHFFFAOYSA-N

Formula: C14H12F3NO4

SMILES: CC(OC(=O)CCC(=O)Oc1ccc(C#N)cc1)C(F)(F)F

Mol. weight [g/mol]: 315.24

Physical Properties

Property code	Value	Unit	Source
gf	-748.91	kJ/mol	Joback Method
hf	-1034.31	kJ/mol	Joback Method
hfus	31.05	kJ/mol	Joback Method
hvap	74.35	kJ/mol	Joback Method
log10ws	-3.87		Crippen Method
logp	2.738		Crippen Method
mcvol	205.930	ml/mol	McGowan Method
pc	1911.91	kPa	Joback Method
rinpol	1912.00		NIST Webbook
rinpol	1912.00		NIST Webbook
tb	800.18	K	Joback Method
tc	1008.78	K	Joback Method
tf	484.98	K	Joback Method
vc	0.823	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	586.93	J/mol×K	800.18	Joback Method
cpg	597.24	J/mol×K	834.95	Joback Method
cpg	606.67	J/mol×K	869.71	Joback Method
cpg	615.27	J/mol×K	904.48	Joback Method
cpg	623.05	J/mol×K	939.25	Joback Method
cpg	630.04	J/mol×K	974.02	Joback Method
cpg	636.28	J/mol×K	1008.78	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389807&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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