Succinic acid, 2,2,3,3,4,4,5,5-octafluoropentyl 4-cyanophenyl ester

Inchi: InChI=1S/C16H11F8NO4/c17-13(18)15(21,22)16(23,24)14(19,20)8-28-11(26)5-6-12(27)

InchiKey: VQCODGTWHZFDLT-UHFFFAOYSA-N

Formula: C16H11F8NO4

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

Mol. weight [g/mol]: 433.25

Physical Properties

Property code	Value	Unit	Source
gf	-1700.44	kJ/mol	Joback Method
hf	-2073.64	kJ/mol	Joback Method
hfus	36.80	kJ/mol	Joback Method
hvap	72.13	kJ/mol	Joback Method
log10ws	-5.19		Crippen Method
logp	3.958		Crippen Method
mcvol	242.960	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2104.00		NIST Webbook
rinpol	2104.00		NIST Webbook
tb	835.83	K	Joback Method
tc	1031.35	K	Joback Method
tf	515.31	K	Joback Method
vc	1.002	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	736.45	J/mol×K	835.83	Joback Method
cpg	745.82	J/mol×K	868.42	Joback Method
cpg	754.40	J/mol×K	901.00	Joback Method
cpg	762.25	J/mol×K	933.59	Joback Method
cpg	769.43	J/mol×K	966.18	Joback Method
cpg	776.00	J/mol×K	998.76	Joback Method
cpg	782.04	J/mol×K	1031.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389809&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