Succinic acid, 2-methylpent-3-yl 4-cyanophenyl ester

Inchi: InChI=1S/C17H21NO4/c1-4-15(12(2)3)22-17(20)10-9-16(19)21-14-7-5-13(11-18)6-8-14/h
InchiKey: DVKCZOWEXANPRY-UHFFFAOYSA-N
Formula: C17H21NO4
SMILES: CCC(OC(=O)CCC(=O)Oc1ccc(C#N)cc1)C(C)C
Mol. weight [g/mol]: 303.35

Physical Properties

Property code	Value	Unit	Source
gf	-144.50	kJ/mol	Joback Method
hf	-504.43	kJ/mol	Joback Method
hfus	33.47	kJ/mol	Joback Method
hvap	84.39	kJ/mol	Joback Method
log10ws	-4.22		Crippen Method
logp	3.222		Crippen Method
mcvol	242.890	ml/mol	McGowan Method
pc	1664.61	kPa	Joback Method
rinpol	2296.00		NIST Webbook
rinpol	2296.00		NIST Webbook
tb	873.80	K	Joback Method
tc	1092.41	K	Joback Method
tf	499.60	K	Joback Method
vc	0.942	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.88	J/mol×K	873.80	Joback Method
cpg	741.38	J/mol×K	910.24	Joback Method
cpg	752.76	J/mol×K	946.67	Joback Method
cpg	763.02	J/mol×K	983.11	Joback Method
cpg	772.18	J/mol×K	1019.54	Joback Method
cpg	780.26	J/mol×K	1055.98	Joback Method
cpg	787.27	J/mol×K	1092.41	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389811&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