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

Inchi: InChI=1S/C16H19NO4/c1-11(2)12(3)20-15(18)8-9-16(19)21-14-6-4-13(10-17)5-7-14/h4-
InchiKey: VYCZYXKHOLMEGE-UHFFFAOYSA-N
Formula: C16H19NO4
SMILES: CC(C)C(C)OC(=O)CCC(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
gf	-152.92	kJ/mol	Joback Method
hf	-483.79	kJ/mol	Joback Method
hfus	30.88	kJ/mol	Joback Method
hvap	82.16	kJ/mol	Joback Method
log10ws	-3.80		Crippen Method
logp	2.832		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinpol	2210.00		NIST Webbook
rinpol	2210.00		NIST Webbook
tb	850.92	K	Joback Method
tc	1070.87	K	Joback Method
tf	488.33	K	Joback Method
vc	0.885	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.57	J/mol×K	850.92	Joback Method
cpg	684.87	J/mol×K	887.58	Joback Method
cpg	696.07	J/mol×K	924.24	Joback Method
cpg	706.19	J/mol×K	960.90	Joback Method
cpg	715.25	J/mol×K	997.55	Joback Method
cpg	723.24	J/mol×K	1034.21	Joback Method
cpg	730.20	J/mol×K	1070.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U389810&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