Succinic acid, 4-cyanophenyl 2-methylbutyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	-150.48	kJ/mol	Joback Method
hf	-478.51	kJ/mol	Joback Method
hfus	34.40	kJ/mol	Joback Method
hvap	82.55	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.833		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	1790.91	kPa	Joback Method
rinpol	2271.00		NIST Webbook
rinpol	2271.00		NIST Webbook
tb	851.36	K	Joback Method
tc	1068.57	K	Joback Method
tf	503.33	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	671.99	J/mol×K	851.36	Joback Method
cpg	684.16	J/mol×K	887.56	Joback Method
cpg	695.27	J/mol×K	923.76	Joback Method
cpg	705.34	J/mol×K	959.97	Joback Method
cpg	714.38	J/mol×K	996.17	Joback Method
cpg	722.40	J/mol×K	1032.37	Joback Method
cpg	729.41	J/mol×K	1068.57	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=U360703&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