Diethylmalonic acid, 4-cyanophenyl pentyl ester

Inchi: InChI=1S/C19H25NO4/c1-4-7-8-13-23-17(21)19(5-2,6-3)18(22)24-16-11-9-15(14-20)10-1

InchiKey: FLMWXYZUQMQDFN-UHFFFAOYSA-N

Formula: C19H25NO4

SMILES: CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C#N)cc1

Mol. weight [g/mol]: 331.41

Physical Properties

Property code	Value	Unit	Source
gf	-119.94	kJ/mol	Joback Method
hf	-543.90	kJ/mol	Joback Method
hfus	38.28	kJ/mol	Joback Method
hvap	88.32	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.003		Crippen Method
mcvol	271.070	ml/mol	McGowan Method
pc	1434.80	kPa	Joback Method
rinpol	2316.00		NIST Webbook
rinpol	2316.00		NIST Webbook
tb	917.21	K	Joback Method
tc	1136.70	K	Joback Method
tf	554.56	K	Joback Method
vc	1.054	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.49	J/mol×K	917.21	Joback Method
cpg	856.34	J/mol×K	953.79	Joback Method
cpg	868.07	J/mol×K	990.37	Joback Method
cpg	878.73	J/mol×K	1026.95	Joback Method
cpg	888.37	J/mol×K	1063.54	Joback Method
cpg	897.02	J/mol×K	1100.12	Joback Method
cpg	904.75	J/mol×K	1136.70	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=U369603&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