Diethylmalonic acid, butyl 4-cyanophenyl ester

Inchi: InChI=1S/C18H23NO4/c1-4-7-12-22-16(20)18(5-2,6-3)17(21)23-15-10-8-14(13-19)9-11-1

InchiKey: CVHYLMZODDJIBO-UHFFFAOYSA-N

Formula: C18H23NO4

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

Mol. weight [g/mol]: 317.38

Physical Properties

Property code	Value	Unit	Source
gf	-128.36	kJ/mol	Joback Method
hf	-523.26	kJ/mol	Joback Method
hfus	35.69	kJ/mol	Joback Method
hvap	86.09	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	3.613		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1545.13	kPa	Joback Method
rinpol	2220.00		NIST Webbook
tb	894.33	K	Joback Method
tc	1114.03	K	Joback Method
tf	543.29	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.82	J/mol×K	894.33	Joback Method
cpg	798.46	J/mol×K	930.95	Joback Method
cpg	810.02	J/mol×K	967.56	Joback Method
cpg	820.53	J/mol×K	1004.18	Joback Method
cpg	830.04	J/mol×K	1040.80	Joback Method
cpg	838.58	J/mol×K	1077.41	Joback Method
cpg	846.21	J/mol×K	1114.03	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369602&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