Diethylmalonic acid, 4-cyanophenyl isobutyl ester

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

InchiKey: YDPZPDZPWONJBS-UHFFFAOYSA-N

Formula: C18H23NO4

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

Mol. weight [g/mol]: 317.38

Physical Properties

Property code	Value	Unit	Source
gf	-130.80	kJ/mol	Joback Method
hf	-528.54	kJ/mol	Joback Method
hfus	32.17	kJ/mol	Joback Method
hvap	85.71	kJ/mol	Joback Method
log10ws	-4.28		Crippen Method
logp	3.469		Crippen Method
mcvol	256.980	ml/mol	McGowan Method
pc	1554.90	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
tb	893.89	K	Joback Method
tc	1115.96	K	Joback Method
tf	528.29	K	Joback Method
vc	0.993	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	786.36	J/mol×K	893.89	Joback Method
cpg	799.10	J/mol×K	930.90	Joback Method
cpg	810.72	J/mol×K	967.91	Joback Method
cpg	821.26	J/mol×K	1004.92	Joback Method
cpg	830.77	J/mol×K	1041.94	Joback Method
cpg	839.27	J/mol×K	1078.95	Joback Method
cpg	846.83	J/mol×K	1115.96	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=U369601&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