Diethylmalonic acid, 4-cyanophenyl undecyl ester

Inchi: InChI=1S/C25H37NO4/c1-4-7-8-9-10-11-12-13-14-19-29-23(27)25(5-2,6-3)24(28)30-22-1

InchiKey: FELHLYGOFIMNCK-UHFFFAOYSA-N

Formula: C25H37NO4

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

Mol. weight [g/mol]: 415.57

Physical Properties

Property code	Value	Unit	Source
gf	-69.42	kJ/mol	Joback Method
hf	-667.74	kJ/mol	Joback Method
hfus	53.82	kJ/mol	Joback Method
hvap	101.68	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.344		Crippen Method
mcvol	355.610	ml/mol	McGowan Method
pc	966.87	kPa	Joback Method
rinpol	2906.00		NIST Webbook
rinpol	2906.00		NIST Webbook
tb	1054.49	K	Joback Method
tc	1291.30	K	Joback Method
tf	622.18	K	Joback Method
vc	1.391	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.46	J/mol×K	1054.49	Joback Method
cpg	1216.59	J/mol×K	1093.96	Joback Method
cpg	1229.34	J/mol×K	1133.43	Joback Method
cpg	1240.79	J/mol×K	1172.89	Joback Method
cpg	1251.03	J/mol×K	1212.36	Joback Method
cpg	1260.13	J/mol×K	1251.83	Joback Method
cpg	1268.17	J/mol×K	1291.30	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U369609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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