Diethylmalonic acid, 4-cyanophenyl decyl ester

Inchi: InChI=1S/C24H35NO4/c1-4-7-8-9-10-11-12-13-18-28-22(26)24(5-2,6-3)23(27)29-21-16-1

InchiKey: FMKQUIGCDGXBPK-UHFFFAOYSA-N

Formula: C24H35NO4

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

Mol. weight [g/mol]: 401.54

Physical Properties

Property code	Value	Unit	Source
gf	-77.84	kJ/mol	Joback Method
hf	-647.10	kJ/mol	Joback Method
hfus	51.23	kJ/mol	Joback Method
hvap	99.45	kJ/mol	Joback Method
log10ws	-7.04		Crippen Method
logp	5.954		Crippen Method
mcvol	341.520	ml/mol	McGowan Method
pc	1027.28	kPa	Joback Method
rinpol	2798.00		NIST Webbook
rinpol	2798.00		NIST Webbook
tb	1031.61	K	Joback Method
tc	1263.02	K	Joback Method
tf	610.91	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.34	J/mol×K	1031.61	Joback Method
cpg	1155.21	J/mol×K	1070.18	Joback Method
cpg	1167.76	J/mol×K	1108.75	Joback Method
cpg	1179.07	J/mol×K	1147.31	Joback Method
cpg	1189.20	J/mol×K	1185.88	Joback Method
cpg	1198.23	J/mol×K	1224.45	Joback Method
cpg	1206.24	J/mol×K	1263.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369608&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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