Diethylmalonic acid, 4-cyanophenyl heptyl ester

Inchi: InChI=1S/C21H29NO4/c1-4-7-8-9-10-15-25-19(23)21(5-2,6-3)20(24)26-18-13-11-17(16-2

InchiKey: BJMXZXIEHGBEIP-UHFFFAOYSA-N

Formula: C21H29NO4

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

Mol. weight [g/mol]: 359.46

Physical Properties

Property code	Value	Unit	Source
gf	-103.10	kJ/mol	Joback Method
hf	-585.18	kJ/mol	Joback Method
hfus	43.46	kJ/mol	Joback Method
hvap	92.77	kJ/mol	Joback Method
log10ws	-5.78		Crippen Method
logp	4.784		Crippen Method
mcvol	299.250	ml/mol	McGowan Method
pc	1246.85	kPa	Joback Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook
tb	962.97	K	Joback Method
tc	1184.47	K	Joback Method
tf	577.10	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	960.89	J/mol×K	962.97	Joback Method
cpg	974.12	J/mol×K	999.89	Joback Method
cpg	986.17	J/mol×K	1036.80	Joback Method
cpg	997.09	J/mol×K	1073.72	Joback Method
cpg	1006.94	J/mol×K	1110.63	Joback Method
cpg	1015.77	J/mol×K	1147.55	Joback Method
cpg	1023.64	J/mol×K	1184.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U369605&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