Diethylmalonic acid, 4-cyanophenyl ethyl ester

Inchi: InChI=1S/C16H19NO4/c1-4-16(5-2,14(18)20-6-3)15(19)21-13-9-7-12(11-17)8-10-13/h7-1
InchiKey: SVAGHCHZBVMBNK-UHFFFAOYSA-N
Formula: C16H19NO4
SMILES: CCOC(=O)C(CC)(CC)C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 289.33

Physical Properties

Property code	Value	Unit	Source
gf	-145.20	kJ/mol	Joback Method
hf	-481.98	kJ/mol	Joback Method
hfus	30.51	kJ/mol	Joback Method
hvap	81.64	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.833		Crippen Method
mcvol	228.800	ml/mol	McGowan Method
pc	1807.70	kPa	Joback Method
rinpol	2054.00		NIST Webbook
rinpol	2054.00		NIST Webbook
tb	848.57	K	Joback Method
tc	1070.88	K	Joback Method
tf	520.75	K	Joback Method
vc	0.886	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	672.81	J/mol×K	848.57	Joback Method
cpg	685.00	J/mol×K	885.62	Joback Method
cpg	696.14	J/mol×K	922.67	Joback Method
cpg	706.28	J/mol×K	959.72	Joback Method
cpg	715.45	J/mol×K	996.77	Joback Method
cpg	723.68	J/mol×K	1033.82	Joback Method
cpg	731.02	J/mol×K	1070.88	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=U369599&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