Diethylmalonic acid, di(4-cyanophenyl) ester

Inchi: InChI=1S/C21H18N2O4/c1-3-21(4-2,19(24)26-17-9-5-15(13-22)6-10-17)20(25)27-18-11-
InchiKey: BDBABQHKCDQJKI-UHFFFAOYSA-N
Formula: C21H18N2O4
SMILES: CCC(CC)(C(=O)Oc1ccc(C#N)cc1)C(=O)Oc1ccc(C#N)cc1
Mol. weight [g/mol]: 362.38

Physical Properties

Property code	Value	Unit	Source
gf	132.86	kJ/mol	Joback Method
hf	-195.24	kJ/mol	Joback Method
hfus	38.62	kJ/mol	Joback Method
hvap	106.19	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	3.747		Crippen Method
mcvol	276.870	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2958.00		NIST Webbook
rinpol	2958.00		NIST Webbook
tb	1096.71	K	Joback Method
tc	1352.81	K	Joback Method
tf	681.03	K	Joback Method
vc	1.085	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	850.30	J/mol×K	1096.71	Joback Method
cpg	857.64	J/mol×K	1139.39	Joback Method
cpg	863.84	J/mol×K	1182.08	Joback Method
cpg	868.99	J/mol×K	1224.76	Joback Method
cpg	873.16	J/mol×K	1267.44	Joback Method
cpg	876.44	J/mol×K	1310.13	Joback Method
cpg	878.91	J/mol×K	1352.81	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=U369610&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