Diethylmalonic acid, 4-nitrophenyl nonyl ester

Inchi: InChI=1S/C22H33NO6/c1-4-7-8-9-10-11-12-17-28-20(24)22(5-2,6-3)21(25)29-19-15-13-1
InchiKey: IWPOEQNKASGOIB-UHFFFAOYSA-N
Formula: C22H33NO6
SMILES: CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 407.50

Physical Properties

Property code	Value	Unit	Source
gf	-192.31	kJ/mol	Joback Method
hf	-781.46	kJ/mol	Joback Method
hfus	55.91	kJ/mol	Joback Method
hvap	101.11	kJ/mol	Joback Method
log10ws	-6.92		Crippen Method
logp	5.600		Crippen Method
mcvol	329.380	ml/mol	McGowan Method
pc	1196.48	kPa	Joback Method
rinpol	2747.00		NIST Webbook
tb	1035.61	K	Joback Method
tc	1269.26	K	Joback Method
tf	666.99	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.71	J/mol×K	1035.61	Joback Method
cpg	1121.83	J/mol×K	1074.55	Joback Method
cpg	1133.63	J/mol×K	1113.49	Joback Method
cpg	1144.19	J/mol×K	1152.43	Joback Method
cpg	1153.59	J/mol×K	1191.37	Joback Method
cpg	1161.90	J/mol×K	1230.32	Joback Method
cpg	1169.20	J/mol×K	1269.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370169&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

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