Diethylmalonic acid, decyl 4-nitrophenyl ester

Inchi: InChI=1S/C23H35NO6/c1-4-7-8-9-10-11-12-13-18-29-21(25)23(5-2,6-3)22(26)30-20-16-1
InchiKey: FXFXOVFGCVFDCZ-UHFFFAOYSA-N
Formula: C23H35NO6
SMILES: CCCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 421.53

Physical Properties

Property code	Value	Unit	Source
gf	-183.89	kJ/mol	Joback Method
hf	-802.10	kJ/mol	Joback Method
hfus	58.50	kJ/mol	Joback Method
hvap	103.34	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.990		Crippen Method
mcvol	343.470	ml/mol	McGowan Method
pc	1120.80	kPa	Joback Method
rinpol	2846.00		NIST Webbook
rinpol	2846.00		NIST Webbook
tb	1058.49	K	Joback Method
tc	1296.08	K	Joback Method
tf	678.26	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1169.40	J/mol×K	1058.49	Joback Method
cpg	1182.69	J/mol×K	1098.09	Joback Method
cpg	1194.62	J/mol×K	1137.69	Joback Method
cpg	1205.27	J/mol×K	1177.28	Joback Method
cpg	1214.73	J/mol×K	1216.88	Joback Method
cpg	1223.09	J/mol×K	1256.48	Joback Method
cpg	1230.42	J/mol×K	1296.08	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=U370170&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