Diethylmalonic acid, 2-nitrophenyl octyl ester

Inchi: InChI=1S/C21H31NO6/c1-4-7-8-9-10-13-16-27-19(23)21(5-2,6-3)20(24)28-18-15-12-11-1
InchiKey: IYPMHGHMPRPPJF-UHFFFAOYSA-N
Formula: C21H31NO6
SMILES: CCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]: 393.47

Physical Properties

Property code	Value	Unit	Source
gf	-200.73	kJ/mol	Joback Method
hf	-760.82	kJ/mol	Joback Method
hfus	53.32	kJ/mol	Joback Method
hvap	98.88	kJ/mol	Joback Method
log10ws	-6.50		Crippen Method
logp	5.210		Crippen Method
mcvol	315.290	ml/mol	McGowan Method
pc	1280.08	kPa	Joback Method
rinpol	2646.00		NIST Webbook
tb	1012.73	K	Joback Method
tc	1243.48	K	Joback Method
tf	655.72	K	Joback Method
vc	1.222	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1048.49	J/mol×K	1012.73	Joback Method
cpg	1061.46	J/mol×K	1051.19	Joback Method
cpg	1073.15	J/mol×K	1089.65	Joback Method
cpg	1083.62	J/mol×K	1128.10	Joback Method
cpg	1092.96	J/mol×K	1166.56	Joback Method
cpg	1101.22	J/mol×K	1205.02	Joback Method
cpg	1108.49	J/mol×K	1243.48	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=U369862&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