Diethylmalonic acid, 2-methylhex-3-yl 4-nitrophenyl ester

Inchi: InChI=1S/C20H29NO6/c1-6-9-17(14(4)5)27-19(23)20(7-2,8-3)18(22)26-16-12-10-15(11-1

InchiKey: XFJRRESISAFVAD-UHFFFAOYSA-N

Formula: C20H29NO6

SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1)C(C)C

Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-214.03	kJ/mol	Joback Method
hf	-750.74	kJ/mol	Joback Method
hfus	43.68	kJ/mol	Joback Method
hvap	95.88	kJ/mol	Joback Method
log10ws	-5.95		Crippen Method
logp	4.675		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1389.18	kPa	Joback Method
rinpol	2419.00		NIST Webbook
rinpol	2419.00		NIST Webbook
tb	988.97	K	Joback Method
tc	1220.88	K	Joback Method
tf	614.45	K	Joback Method
vc	1.155	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	989.59	J/mol×K	988.97	Joback Method
cpg	1002.45	J/mol×K	1027.62	Joback Method
cpg	1014.00	J/mol×K	1066.27	Joback Method
cpg	1024.31	J/mol×K	1104.92	Joback Method
cpg	1033.44	J/mol×K	1143.57	Joback Method
cpg	1041.45	J/mol×K	1182.23	Joback Method
cpg	1048.42	J/mol×K	1220.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370165&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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