Diethylmalonic acid, heptyl 4-nitrophenyl ester

Inchi: InChI=1S/C20H29NO6/c1-4-7-8-9-10-15-26-18(22)20(5-2,6-3)19(23)27-17-13-11-16(12-1
InchiKey: FTCQMVXJOQPOPS-UHFFFAOYSA-N
Formula: C20H29NO6
SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 379.45

Physical Properties

Property code	Value	Unit	Source
gf	-209.15	kJ/mol	Joback Method
hf	-740.18	kJ/mol	Joback Method
hfus	50.73	kJ/mol	Joback Method
hvap	96.66	kJ/mol	Joback Method
log10ws	-6.08		Crippen Method
logp	4.820		Crippen Method
mcvol	301.200	ml/mol	McGowan Method
pc	1372.76	kPa	Joback Method
rinpol	2555.00		NIST Webbook
tb	989.85	K	Joback Method
tc	1218.67	K	Joback Method
tf	644.45	K	Joback Method
vc	1.167	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	988.78	J/mol×K	989.85	Joback Method
cpg	1001.61	J/mol×K	1027.99	Joback Method
cpg	1013.19	J/mol×K	1066.12	Joback Method
cpg	1023.58	J/mol×K	1104.26	Joback Method
cpg	1032.86	J/mol×K	1142.40	Joback Method
cpg	1041.08	J/mol×K	1180.54	Joback Method
cpg	1048.30	J/mol×K	1218.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370167&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