

Diethylmalonic acid, 4-nitrophenyl pentyl ester

Inchi:	InChI=1S/C18H25NO6/c1-4-7-8-13-24-16(20)18(5-2,6-3)17(21)25-15-11-9-14(10-12-15)
InchiKey:	JCDGKFFIGAKQPS-UHFFFAOYSA-N
Formula:	C18H25NO6
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	351.39

Physical Properties

Property code	Value	Unit	Source
gf	-225.99	kJ/mol	Joback Method
hf	-698.90	kJ/mol	Joback Method
hfus	45.55	kJ/mol	Joback Method
hvap	92.21	kJ/mol	Joback Method
log10ws	-5.24		Crippen Method
logp	4.040		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1591.08	kPa	Joback Method
rinsol	2363.00		NIST Webbook
tb	944.09	K	Joback Method
tc	1171.77	K	Joback Method
tf	621.91	K	Joback Method
vc	1.054	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	871.04	J/molxK	944.09	Joback Method
cpg	883.61	J/molxK	982.04	Joback Method
cpg	894.98	J/molxK	1019.98	Joback Method
cpg	905.20	J/molxK	1057.93	Joback Method
cpg	914.34	J/molxK	1095.88	Joback Method
cpg	922.43	J/molxK	1133.82	Joback Method
cpg	929.55	J/molxK	1171.77	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=U370164&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	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

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