(Z)-Dec-4-enyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C17H22N2O6/c1-2-3-4-5-6-7-8-9-10-25-17(20)14-11-15(18(21)22)13-16(12-14
InchiKey: MGPJETGWCBDIKR-SREVYHEPSA-N
Formula: C17H22N2O6
SMILES: CCCCCC=CCCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 350.37

Physical Properties

Property code	Value	Unit	Source
gf	102.81	kJ/mol	Joback Method
hf	-329.72	kJ/mol	Joback Method
hfus	58.76	kJ/mol	Joback Method
hvap	99.33	kJ/mol	Joback Method
log10ws	-6.64		Crippen Method
logp	4.576		Crippen Method
mcvol	264.610	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2626.00		NIST Webbook
tb	1009.13	K	Joback Method
tc	1250.96	K	Joback Method
tf	687.11	K	Joback Method
vc	1.048	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.88	J/mol×K	1009.13	Joback Method
cpg	855.21	J/mol×K	1049.43	Joback Method
cpg	865.52	J/mol×K	1089.74	Joback Method
cpg	874.90	J/mol×K	1130.04	Joback Method
cpg	883.42	J/mol×K	1170.35	Joback Method
cpg	891.15	J/mol×K	1210.65	Joback Method
cpg	898.17	J/mol×K	1250.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373872&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