(Z)-Non-3-enyl 3,5-dinitrobenzoate

Inchi: InChI=1S/C16H20N2O6/c1-2-3-4-5-6-7-8-9-24-16(19)13-10-14(17(20)21)12-15(11-13)18
InchiKey: NGPMTKXASHVMHN-SREVYHEPSA-N
Formula: C16H20N2O6
SMILES: CCCCCC=CCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 336.34

Physical Properties

Property code	Value	Unit	Source
gf	94.39	kJ/mol	Joback Method
hf	-309.08	kJ/mol	Joback Method
hfus	56.17	kJ/mol	Joback Method
hvap	97.11	kJ/mol	Joback Method
log10ws	-6.22		Crippen Method
logp	4.186		Crippen Method
mcvol	250.520	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpol	2525.00		NIST Webbook
tb	986.25	K	Joback Method
tc	1228.93	K	Joback Method
tf	675.84	K	Joback Method
vc	0.992	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	785.69	J/mol×K	986.25	Joback Method
cpg	796.78	J/mol×K	1026.70	Joback Method
cpg	806.88	J/mol×K	1067.14	Joback Method
cpg	816.04	J/mol×K	1107.59	Joback Method
cpg	824.34	J/mol×K	1148.04	Joback Method
cpg	831.85	J/mol×K	1188.49	Joback Method
cpg	838.65	J/mol×K	1228.93	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373860&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

Latest version available from:
https://www.chemeo.com/cid/13-820-6/Z-Non-3-enyl-3-5-dinitrobenzoate.pdf
Generated by Cheméo on 2024-04-26 05:15:19.945545376 +0000 UTC m=+16397768.866122691.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.