(E)-Hex-3-enyl 3,5-dinitrobenzoate

Other names: Benzoic acid, 3,5-dinitro, (E)-3-hexenyl ester
(E)-3-Hexenyl 3,5-dinitrobenzoate
Inchi: InChI=1S/C13H14N2O6/c1-2-3-4-5-6-21-13(16)10-7-11(14(17)18)9-12(8-10)15(19)20/h3
InchiKey: QVOVOBIUXJFNNO-ONEGZZNKSA-N
Formula: C13H14N2O6
SMILES: CCC=CCCOC(=O)c1cc([N+](=O)[O-])cc([N+](=O)[O-])c1
Mol. weight [g/mol]: 294.26

Physical Properties

Property code	Value	Unit	Source
gf	69.13	kJ/mol	Joback Method
hf	-247.16	kJ/mol	Joback Method
hfus	48.40	kJ/mol	Joback Method
hvap	90.43	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	3.016		Crippen Method
mcvol	208.250	ml/mol	McGowan Method
pc	2395.87	kPa	Joback Method
rinpol	2144.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2156.00		NIST Webbook
rinpol	2119.00		NIST Webbook
rinpol	2134.00		NIST Webbook
ripol	3104.00		NIST Webbook
ripol	3125.00		NIST Webbook
ripol	3084.00		NIST Webbook
ripol	3116.00		NIST Webbook
tb	917.61	K	Joback Method
tc	1167.80	K	Joback Method
tf	642.03	K	Joback Method
vc	0.824	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.41	J/mol×K	917.61	Joback Method
cpg	625.70	J/mol×K	959.31	Joback Method
cpg	635.02	J/mol×K	1001.01	Joback Method
cpg	643.41	J/mol×K	1042.70	Joback Method
cpg	650.96	J/mol×K	1084.40	Joback Method
cpg	657.70	J/mol×K	1126.10	Joback Method
cpg	663.72	J/mol×K	1167.80	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373867&Units=SI

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume