

Benzoic acid, 4-nitro, (E)-3-hexenyl ester

Other names:	(E)-3-Hexenyl 4-nitrobenzoate
Inchi:	InChI=1S/C13H15NO4/c1-2-3-4-5-10-18-13(15)11-6-8-12(9-7-11)14(16)17/h3-4,6-9H,2,5
InchiKey:	AGMSPQYTEWLJLC-ONEGZZNKSA-N
Formula:	C13H15NO4
SMILES:	CCC=CCCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	249.26

Physical Properties

Property code	Value	Unit	Source
gf	43.21	kJ/mol	Joback Method
hf	-224.93	kJ/mol	Joback Method
hfus	37.43	kJ/mol	Joback Method
hvap	73.18	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.108		Crippen Method
mcvol	190.830	ml/mol	McGowan Method
pc	2402.92	kPa	Joback Method
rinpol	1904.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1897.00		NIST Webbook
rinpol	1907.00		NIST Webbook
ripol	2718.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2701.00		NIST Webbook
ripol	2706.00		NIST Webbook
ripol	2739.00		NIST Webbook
tb	760.79	K	Joback Method
tc	993.55	K	Joback Method
tf	485.90	K	Joback Method
vc	0.742	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cpg	525.56	J/mol×K	760.79	Joback Method
cpg	538.62	J/mol×K	799.58	Joback Method
cpg	550.70	J/mol×K	838.38	Joback Method
cpg	561.86	J/mol×K	877.17	Joback Method
cpg	572.13	J/mol×K	915.96	Joback Method
cpg	581.57	J/mol×K	954.76	Joback Method
cpg	590.24	J/mol×K	993.55	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=R34806&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

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