

Benzoic acid, 4-nitro, allyl ester

Other names:	2-Propenyl 4-nitrobenzoate
Inchi:	InChI=1S/C10H9NO4/c1-2-7-15-10(12)8-3-5-9(6-4-8)11(13)14/h2-6H,1,7H2
InchiKey:	FNAOSVAQWXBRLK-UHFFFAOYSA-N
Formula:	C10H9NO4
SMILES:	C=CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	207.18

Physical Properties

Property code	Value	Unit	Source
gf	25.57	kJ/mol	Joback Method
hf	-154.80	kJ/mol	Joback Method
hfus	28.18	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-3.06		Crippen Method
logp	1.938		Crippen Method
mcvol	148.560	ml/mol	McGowan Method
pc	3220.98	kPa	Joback Method
rinpol	1580.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1577.00		NIST Webbook
ripol	2446.00		NIST Webbook
ripol	2428.00		NIST Webbook
ripol	2446.00		NIST Webbook
ripol	2486.00		NIST Webbook
ripol	2458.00		NIST Webbook
ripol	2428.00		NIST Webbook
tb	684.67	K	Joback Method
tc	926.88	K	Joback Method
tf	455.41	K	Joback Method
vc	0.575	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.22	J/molxK	684.67	Joback Method
cpg	383.64	J/molxK	725.04	Joback Method
cpg	394.14	J/molxK	765.41	Joback Method
cpg	403.77	J/molxK	805.77	Joback Method
cpg	412.56	J/molxK	846.14	Joback Method
cpg	420.54	J/molxK	886.51	Joback Method
cpg	427.74	J/molxK	926.88	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34664&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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