

Benzoic acid, 4-nitro, (E)-2-butenyl ester

Other names:	(E)-2-Butenyl 4-nitrobenzoate
Inchi:	InChI=1S/C11H11NO4/c1-2-3-8-16-11(13)9-4-6-10(7-5-9)12(14)15/h2-7H,8H2,1H3/b3-2
InchiKey:	IFYMPHLEENWYIT-NSCUHMNNSA-N
Formula:	C11H11NO4
SMILES:	CC=CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	221.21

Physical Properties

Property code	Value	Unit	Source
gf	26.37	kJ/mol	Joback Method
hf	-183.65	kJ/mol	Joback Method
hfus	32.25	kJ/mol	Joback Method
hvap	68.72	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.328		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	1709.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1728.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1709.00		NIST Webbook
ripol	2586.00		NIST Webbook
ripol	2562.00		NIST Webbook
ripol	2569.00		NIST Webbook
ripol	2562.00		NIST Webbook
ripol	2606.00		NIST Webbook
ripol	2569.00		NIST Webbook
tb	715.03	K	Joback Method
tc	956.93	K	Joback Method
tf	463.36	K	Joback Method
vc	0.629	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.70	J/molxK	715.03	Joback Method
cpg	433.77	J/molxK	755.35	Joback Method
cpg	444.88	J/molxK	795.66	Joback Method
cpg	455.10	J/molxK	835.98	Joback Method
cpg	464.47	J/molxK	876.29	Joback Method
cpg	473.04	J/molxK	916.61	Joback Method
cpg	480.85	J/molxK	956.93	Joback Method

Sources

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=R34771&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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