Benzoic acid, 4-nitro, 3-butenyl ester

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

Physical Properties

Property code	Value	Unit	Source
gf	33.99	kJ/mol	Joback Method
hf	-175.44	kJ/mol	Joback Method
hfus	30.77	kJ/mol	Joback Method
hvap	68.09	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.328		Crippen Method
mcvol	162.650	ml/mol	McGowan Method
pc	2896.73	kPa	Joback Method
rinpol	1675.00		NIST Webbook
rinpol	1678.00		NIST Webbook
ripol	2529.00		NIST Webbook
ripol	2522.00		NIST Webbook
tb	707.55	K	Joback Method
tc	944.79	K	Joback Method
tf	466.68	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.09	J/mol×K	707.55	Joback Method
cpg	434.15	J/mol×K	747.09	Joback Method
cpg	445.26	J/mol×K	786.63	Joback Method
cpg	455.47	J/mol×K	826.17	Joback Method
cpg	464.81	J/mol×K	865.71	Joback Method

cpg	473.32	J/mol×K	905.25	Joback Method
cpg	481.02	J/mol×K	944.79	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R34717&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

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