Benzoic acid, 4-nitro, 1-methyl-3-butenyl ester

Other names: 4-Penten-2-yl 4-nitrobenzoate
Inchi: InChI=1S/C12H13NO4/c1-3-4-9(2)17-12(14)10-5-7-11(8-6-10)13(15)16/h3,5-9H,1,4H2,2
InchiKey: XOURINZFXLPYEX-UHFFFAOYSA-N
Formula: C12H13NO4
SMILES: C=CCC(C)OC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 235.24

Physical Properties

Property code	Value	Unit	Source
gf	39.97	kJ/mol	Joback Method
hf	-201.36	kJ/mol	Joback Method
hfus	29.83	kJ/mol	Joback Method
hvap	69.93	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	2.716		Crippen Method
mcvol	176.740	ml/mol	McGowan Method
pc	2640.67	kPa	Joback Method
rinpol	1706.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1706.00		NIST Webbook
rinpol	1716.00		NIST Webbook
rinpol	1708.00		NIST Webbook
rinpol	1728.00		NIST Webbook
ripol	2511.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2498.00		NIST Webbook
ripol	2484.00		NIST Webbook
ripol	2538.00		NIST Webbook
ripol	2498.00		NIST Webbook
tb	729.99	K	Joback Method
tc	967.12	K	Joback Method
tf	462.95	K	Joback Method
vc	0.680	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	473.87	J/mol×K	729.99	Joback Method
cpg	486.72	J/mol×K	769.51	Joback Method
cpg	498.55	J/mol×K	809.03	Joback Method
cpg	509.40	J/mol×K	848.56	Joback Method
cpg	519.31	J/mol×K	888.08	Joback Method
cpg	528.33	J/mol×K	927.60	Joback Method
cpg	536.48	J/mol×K	967.12	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=R34735&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