Benzoic acid, 4-nitro, 2-propynyl ester

Other names: 2-Propynyl 4-nitrobenzoate
Inchi: InChI=1S/C10H7NO4/c1-2-7-15-10(12)8-3-5-9(6-4-8)11(13)14/h1,3-6H,7H2
InchiKey: GFKCCMNDZCDTGK-UHFFFAOYSA-N
Formula: C10H7NO4
SMILES: C#CCOC(=O)c1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 205.17

Physical Properties

Property code	Value	Unit	Source
gf	160.80	kJ/mol	Joback Method
hf	11.67	kJ/mol	Joback Method
hfus	32.43	kJ/mol	Joback Method
hvap	66.40	kJ/mol	Joback Method
log10ws	-3.00		Crippen Method
logp	1.385		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
pc	3646.53	kPa	Joback Method
rinpol	1593.00		NIST Webbook
rinpol	1587.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1587.00		NIST Webbook
ripol	2644.00		NIST Webbook
ripol	2644.00		NIST Webbook
ripol	2644.00		NIST Webbook
ripol	2672.00		NIST Webbook
ripol	2661.00		NIST Webbook
tb	678.11	K	Joback Method
tc	932.23	K	Joback Method
tf	504.14	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	349.65	J/mol×K	678.11	Joback Method
cpg	360.29	J/mol×K	720.46	Joback Method
cpg	370.02	J/mol×K	762.82	Joback Method
cpg	378.90	J/mol×K	805.17	Joback Method
cpg	386.96	J/mol×K	847.52	Joback Method
cpg	394.23	J/mol×K	889.88	Joback Method
cpg	400.76	J/mol×K	932.23	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R34682&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