

Benzenebutanoic acid, 4-nitro-, methyl ester

Other names:	Butyric acid, 4-(p-nitrophenyl)-, methyl ester Methyl 4-(4-nitrophenyl)butanoate 4-(4-Nitrophenyl)butanoic acid methyl ester
Inchi:	InChI=1S/C11H13NO4/c1-16-11(13)4-2-3-9-5-7-10(8-6-9)12(14)15/h5-8H,2-4H2,1H3
InchiKey:	IIDUVWAKHMUVPN-UHFFFAOYSA-N
Formula:	C11H13NO4
SMILES:	COC(=O)CCCC1=CC=C([N+](=O)[O-])C=C1
Mol. weight [g/mol]:	223.23
CAS:	20637-02-9

Physical Properties

Property code	Value	Unit	Source
gf	-53.85	kJ/mol	Joback Method
hf	-300.87	kJ/mol	Joback Method
hfus	32.05	kJ/mol	Joback Method
hvap	68.77	kJ/mol	Joback Method
ie	9.30 ± 0.20	eV	NIST Webbook
ie	8.90 ± 0.30	eV	NIST Webbook
log10ws	-3.04		Crippen Method
logp	2.091		Crippen Method
mcvol	166.950	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	710.87	K	Joback Method
tc	943.55	K	Joback Method
tf	468.44	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.69	J/molxK	710.87	Joback Method
cpg	458.43	J/molxK	749.65	Joback Method
cpg	470.23	J/molxK	788.43	Joback Method
cpg	481.10	J/molxK	827.21	Joback Method

cpg	491.07	J/mol×K	865.99	Joback Method
cpg	500.18	J/mol×K	904.77	Joback Method
cpg	508.44	J/mol×K	943.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20637029&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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