

Butanoic acid, 4-nitro-, methyl ester

Other names:	Butyric acid, 4-nitro-, methyl ester Methyl 4-nitrobutyrate 4-Nitrobutyric acid methyl ester
Inchi:	InChI=1S/C5H9NO4/c1-10-5(7)3-2-4-6(8)9/h2-4H2,1H3
InchiKey:	UBSPKGKFFQKZJB-UHFFFAOYSA-N
Formula:	C5H9NO4
SMILES:	COC(=O)CCC[N+](=O)[O-]
Mol. weight [g/mol]:	147.13
CAS:	13013-02-0

Physical Properties

Property code	Value	Unit	Source
gf	-207.15	kJ/mol	Joback Method
hf	-402.09	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	52.47	kJ/mol	Joback Method
log10ws	-0.86		Crippen Method
logp	0.216		Crippen Method
mcvol	106.170	ml/mol	McGowan Method
pc	3718.02	kPa	Joback Method
tb	541.93	K	Joback Method
tc	754.03	K	Joback Method
tf	361.88	K	Joback Method
vc	0.421	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.45	J/molxK	541.93	Joback Method
cpg	253.02	J/molxK	577.28	Joback Method
cpg	262.11	J/molxK	612.63	Joback Method
cpg	270.73	J/molxK	647.98	Joback Method
cpg	278.88	J/molxK	683.33	Joback Method
cpg	286.56	J/molxK	718.68	Joback Method

cpg

293.77

J/mol×K

754.03

Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	381.20	K	1.00	NIST Webbook

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=C13013020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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