

Benzeneethanol, 3-nitro-

Other names:	«beta»-(m-Nitrophenyl)ethanol 3-Nitrobenzeneethanol 3-Nitrophenethyl alcohol m-nitrophenethyl alcohol
Inchi:	InChI=1S/C8H9NO3/c10-5-4-7-2-1-3-8(6-7)9(11)12/h1-3,6,10H,4-5H2
InchiKey:	PWZWTSYUZQZFKE-UHFFFAOYSA-N
Formula:	C8H9NO3
SMILES:	O=[N+](O)c1cccc(CCO)c1
Mol. weight [g/mol]:	167.16
CAS:	52022-77-2

Physical Properties

Property code	Value	Unit	Source
gf	17.99	kJ/mol	Joback Method
hf	-146.38	kJ/mol	Joback Method
hfus	25.58	kJ/mol	Joback Method
hvap	69.61	kJ/mol	Joback Method
log10ws	-2.19		Crippen Method
logp	1.130		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4077.71	kPa	Joback Method
tb	658.12	K	Joback Method
tc	881.82	K	Joback Method
tf	423.29	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.91	J/molxK	658.12	Joback Method
cpg	318.61	J/molxK	695.40	Joback Method
cpg	327.62	J/molxK	732.69	Joback Method
cpg	335.99	J/molxK	769.97	Joback Method
cpg	343.74	J/molxK	807.26	Joback Method

cpg	350.92	J/mol×K	844.54	Joback Method
cpg	357.55	J/mol×K	881.82	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	416.70	K	0.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C52022772&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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