1-(Nitromethyl)-cyclohexanol

Other names: 1-Nitromethyl-1-cyclohexanol
Inchi: InChI=1S/C7H13NO3/c9-7(6-8(10)11)4-2-1-3-5-7/h9H,1-6H2
InchiKey: WYXVEDWVPJRBJM-UHFFFAOYSA-N
Formula: C7H13NO3
SMILES: O=[N+]([O-])CC1(O)CCCCC1
Mol. weight [g/mol]: 159.18
CAS: 3164-73-6

Physical Properties

Property code	Value	Unit	Source
gf	-74.25	kJ/mol	Joback Method
hf	-281.24	kJ/mol	Joback Method
hfus	14.87	kJ/mol	Joback Method
hvap	63.72	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	0.958		Crippen Method
mcvol	121.920	ml/mol	McGowan Method
pc	4238.55	kPa	Joback Method
tb	623.37	K	Joback Method
tc	851.86	K	Joback Method
tf	404.36	K	Joback Method
vc	0.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	329.53	J/mol×K	623.37	Joback Method
cpg	342.34	J/mol×K	661.45	Joback Method
cpg	354.36	J/mol×K	699.53	Joback Method
cpg	365.75	J/mol×K	737.61	Joback Method
cpg	376.64	J/mol×K	775.70	Joback Method
cpg	387.16	J/mol×K	813.78	Joback Method
cpg	397.44	J/mol×K	851.86	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	407.50 ± 1.50	K	2.90	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3164736&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
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