4-Methyl-3-nitrobenzyl alcohol

Other names: Benzenemethanol, 4-methyl-3-nitro-
Inchi: InChI=1S/C8H9NO3/c1-6-2-3-7(5-10)4-8(6)9(11)12/h2-4,10H,5H2,1H3
InchiKey: URCWIFSXDARYLY-UHFFFAOYSA-N
Formula: C8H9NO3
SMILES: Cc1ccc(CO)cc1[N+](=O)[O-]
Mol. weight [g/mol]: 167.16
CAS: 40870-59-5

Physical Properties

Property code	Value	Unit	Source
gf	8.36	kJ/mol	Joback Method
hf	-157.85	kJ/mol	Joback Method
hfus	25.19	kJ/mol	Joback Method
hvap	70.27	kJ/mol	Joback Method
log10ws	-2.74		Crippen Method
logp	1.396		Crippen Method
mcvol	123.110	ml/mol	McGowan Method
pc	4000.70	kPa	Joback Method
tb	663.10	K	Joback Method
tc	887.68	K	Joback Method
tf	435.81	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.32	J/mol×K	663.10	Joback Method
cpg	316.86	J/mol×K	700.53	Joback Method
cpg	325.75	J/mol×K	737.96	Joback Method
cpg	334.03	J/mol×K	775.39	Joback Method
cpg	341.72	J/mol×K	812.82	Joback Method
cpg	348.85	J/mol×K	850.25	Joback Method
cpg	355.45	J/mol×K	887.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40870595&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume