3-(4-Nitroanilino)-1-propanol

Inchi: InChI=1S/C9H12N2O3/c12-7-1-6-10-8-2-4-9(5-3-8)11(13)14/h2-5,10,12H,1,6-7H2
InchiKey: WVKYZNIVNCTAQE-UHFFFAOYSA-N
Formula: C9H12N2O3
SMILES: O=[N+]([O-])c1ccc(NCCCO)cc1
Mol. weight [g/mol]: 196.20
CAS: 86651-99-2

Physical Properties

Property code	Value	Unit	Source
gf	115.80	kJ/mol	Joback Method
hf	-113.55	kJ/mol	Joback Method
hfus	33.27	kJ/mol	Joback Method
hvap	78.27	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.389		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3677.55	kPa	Joback Method
tb	731.17	K	Joback Method
tc	949.97	K	Joback Method
tf	348.70 ± 0.20	K	NIST Webbook
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.02	J/mol×K	731.17	Joback Method
cpg	414.22	J/mol×K	767.64	Joback Method
cpg	423.70	J/mol×K	804.10	Joback Method
cpg	432.49	J/mol×K	840.57	Joback Method
cpg	440.64	J/mol×K	877.04	Joback Method
cpg	448.18	J/mol×K	913.51	Joback Method
cpg	455.16	J/mol×K	949.97	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86651992&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