3-Nitrobenzyl alcohol, 1-methylpropyl ether

Inchi: InChI=1S/C11H15NO3/c1-3-9(2)15-8-10-5-4-6-11(7-10)12(13)14/h4-7,9H,3,8H2,1-2H3
InchiKey: QQSJAWUYUJQDQM-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: CCC(C)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 209.24

Physical Properties

Property code	Value	Unit	Source
gf	72.63	kJ/mol	Joback Method
hf	-193.57	kJ/mol	Joback Method
hfus	26.92	kJ/mol	Joback Method
hvap	61.63	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	2.910		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
rinpol	1652.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	656.56	K	Joback Method
tc	887.95	K	Joback Method
tf	403.51	K	Joback Method
vc	0.637	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.40	J/mol×K	656.56	Joback Method
cpg	447.06	J/mol×K	695.12	Joback Method
cpg	460.73	J/mol×K	733.69	Joback Method
cpg	473.45	J/mol×K	772.25	Joback Method
cpg	485.23	J/mol×K	810.82	Joback Method
cpg	496.12	J/mol×K	849.38	Joback Method
cpg	506.13	J/mol×K	887.95	Joback Method

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=U374922&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume