(3-Nitrophenyl) methanol, n-butyl ether

Inchi: InChI=1S/C11H15NO3/c1-2-3-7-15-9-10-5-4-6-11(8-10)12(13)14/h4-6,8H,2-3,7,9H2,1H3
InchiKey: RXQSZDVLVTUWCQ-UHFFFAOYSA-N
Formula: C11H15NO3
SMILES: CCCCOCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 209.24

Physical Properties

Property code	Value	Unit	Source
gf	75.07	kJ/mol	Joback Method
hf	-188.29	kJ/mol	Joback Method
hfus	30.45	kJ/mol	Joback Method
hvap	62.02	kJ/mol	Joback Method
log10ws	-3.76		Crippen Method
logp	2.911		Crippen Method
mcvol	165.380	ml/mol	McGowan Method
pc	2595.13	kPa	Joback Method
rinpol	1700.00		NIST Webbook
tb	657.00	K	Joback Method
tc	883.75	K	Joback Method
tf	418.51	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.88	J/mol×K	657.00	Joback Method
cpg	446.22	J/mol×K	694.79	Joback Method
cpg	459.61	J/mol×K	732.58	Joback Method
cpg	472.10	J/mol×K	770.38	Joback Method
cpg	483.70	J/mol×K	808.17	Joback Method
cpg	494.45	J/mol×K	845.96	Joback Method
cpg	504.37	J/mol×K	883.75	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374646&Units=SI

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