(3-Nitrophenyl) methanol, n-propyl ether

Inchi: InChI=1S/C10H13NO3/c1-2-6-14-8-9-4-3-5-10(7-9)11(12)13/h3-5,7H,2,6,8H2,1H3
InchiKey: JSBSRQZVRQKUFP-UHFFFAOYSA-N
Formula: C10H13NO3
SMILES: CCCOCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 195.22

Physical Properties

Property code	Value	Unit	Source
gf	66.65	kJ/mol	Joback Method
hf	-167.65	kJ/mol	Joback Method
hfus	27.86	kJ/mol	Joback Method
hvap	59.79	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	2.521		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
rinpol	1597.00		NIST Webbook
rinpol	1597.00		NIST Webbook
tb	634.12	K	Joback Method
tc	865.31	K	Joback Method
tf	407.24	K	Joback Method
vc	0.588	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	382.25	J/mol×K	634.12	Joback Method
cpg	395.94	J/mol×K	672.65	Joback Method
cpg	408.72	J/mol×K	711.18	Joback Method
cpg	420.63	J/mol×K	749.72	Joback Method
cpg	431.69	J/mol×K	788.25	Joback Method
cpg	441.93	J/mol×K	826.78	Joback Method
cpg	451.36	J/mol×K	865.31	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374645&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume