(3-Nitrophenyl) methanol, n-pentyl ether

Inchi: InChI=1S/C12H17NO3/c1-2-3-4-8-16-10-11-6-5-7-12(9-11)13(14)15/h5-7,9H,2-4,8,10H2
InchiKey: MLJRNALFNDLSOC-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: CCCCCOCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 223.27

Physical Properties

Property code	Value	Unit	Source
gf	83.49	kJ/mol	Joback Method
hf	-208.93	kJ/mol	Joback Method
hfus	33.04	kJ/mol	Joback Method
hvap	64.25	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.302		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1804.00		NIST Webbook
rinpol	1804.00		NIST Webbook
tb	679.88	K	Joback Method
tc	902.53	K	Joback Method
tf	429.78	K	Joback Method
vc	0.700	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	482.95	J/mol×K	679.88	Joback Method
cpg	497.82	J/mol×K	716.99	Joback Method
cpg	511.73	J/mol×K	754.10	Joback Method
cpg	524.70	J/mol×K	791.21	Joback Method
cpg	536.76	J/mol×K	828.32	Joback Method
cpg	547.94	J/mol×K	865.42	Joback Method
cpg	558.27	J/mol×K	902.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U374650&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

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