(3-Nitrophenyl) methanol, 3-methylbutyl ether

Inchi: InChI=1S/C12H17NO3/c1-10(2)6-7-16-9-11-4-3-5-12(8-11)13(14)15/h3-5,8,10H,6-7,9H2
InchiKey: RUNUPAYXCRHBDZ-UHFFFAOYSA-N
Formula: C12H17NO3
SMILES: CC(C)CCOCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]: 223.27

Physical Properties

Property code	Value	Unit	Source
gf	81.05	kJ/mol	Joback Method
hf	-214.21	kJ/mol	Joback Method
hfus	29.51	kJ/mol	Joback Method
hvap	63.86	kJ/mol	Joback Method
log10ws	-3.94		Crippen Method
logp	3.158		Crippen Method
mcvol	179.470	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1762.00		NIST Webbook
tb	679.44	K	Joback Method
tc	906.44	K	Joback Method
tf	414.78	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.47	J/mol×K	679.44	Joback Method
cpg	498.67	J/mol×K	717.27	Joback Method
cpg	512.84	J/mol×K	755.11	Joback Method
cpg	526.03	J/mol×K	792.94	Joback Method
cpg	538.27	J/mol×K	830.77	Joback Method
cpg	549.58	J/mol×K	868.61	Joback Method
cpg	559.99	J/mol×K	906.44	Joback Method

Sources

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=U374648&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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