Butyl 4-nitrophenyl ether

Other names:	p-Nitrophenyl butyl ether
	n-Butyl 4-nitrophenyl ether
	p-Butoxynitrobenzene
	4-n-Butoxynitrobenzene
Inchi:	InChI=1S/C10H13NO3/c1-2-3-8-14-10-6-4-9(5-7-10)11(12)13/h4-7H,2-3,8H2,1H3
InchiKey:	XCCDVVZINDJESR-UHFFFAOYSA-N
Formula:	C10H13NO3
SMILES:	CCCCOc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]:	195.22
CAS:	7244-78-2

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	-3.50		Crippen Method
logp	2.774		Crippen Method
mcvol	151.290	ml/mol	McGowan Method
pc	2868.87	kPa	Joback Method
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	447.50 ± 0.50	K	2.00	NIST Webbook

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=C7244782&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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