p-Nitrobutylbenzene

Other names: 1-butyl-4-nitrobenzene
Inchi: InChI=1S/C10H13NO2/c1-2-3-4-9-5-7-10(8-6-9)11(12)13/h5-8H,2-4H2,1H3
InchiKey: JZRBCNLSIDKBMG-UHFFFAOYSA-N
Formula: C10H13NO2
SMILES: CCCCc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 179.22
CAS: 20651-75-6

Physical Properties

Property code	Value	Unit	Source
af	0.5978		Cheméo Relay (1.0)
gf	171.65	kJ/mol	Joback Method
hf	-30.70	kJ/mol	Cheméo Relay (1.0)
hfus	26.67	kJ/mol	Joback Method
hvap	71.88	kJ/mol	Cheméo Relay (1.0)
ie	10.10 ± 0.10	eV	NIST Webbook
log10ws	-4.26		Cheméo Relay (1.0)
logp	2.937		Crippen Method
mcvol	145.420	ml/mol	McGowan Method
pc	2921.84	kPa	Joback Method
ripol	2234.00		NIST Webbook
ripol	2234.00		NIST Webbook
tb	549.12	K	Cheméo Relay (1.0)
tc	773.03	K	Cheméo Relay (1.0)
tf	278.41	K	Cheméo Relay (1.0)
vc	0.520	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	358.03	J/mol×K	611.70	Joback Method
cpg	372.01	J/mol×K	650.80	Joback Method
cpg	385.03	J/mol×K	689.90	Joback Method
cpg	397.15	J/mol×K	728.99	Joback Method

cpg	408.40	J/mol×K	768.09	Joback Method
cpg	418.84	J/mol×K	807.19	Joback Method
cpg	428.50	J/mol×K	846.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.20	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.19846e+01
Coeff. B	-3.48795e+03
Coeff. C	-8.13960e+01
Temperature range (K), min.	379.59
Temperature range (K), max.	604.08

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20651756&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af:	Acentric Factor
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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume