1-BUTYL-3-PHENYLUREA

Other names: Urea, N-butyl-N'-phenyl-
Inchi: InChI=1S/C11H16N2O/c1-2-3-9-12-11(14)13-10-7-5-4-6-8-10/h4-8H,2-3,9H2,1H3,(H2,12
InchiKey: DOUCJWNVCGEZRR-UHFFFAOYSA-N
Formula: C11H16N2O
SMILES: CCCCNC(=O)Nc1ccccc1
Mol. weight [g/mol]: 192.26

Physical Properties

Property code	Value	Unit	Source
hf	-182.89	kJ/mol	Cheméo Relay (1.0)
hfus	30.08	kJ/mol	Joback Method
hvap	79.56	kJ/mol	Cheméo Relay (1.0)
ie	8.21	eV	Cheméo Relay (1.0)
log10ws	-3.11		Cheméo Relay (1.0)
logp	2.608		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2909.25	kPa	Joback Method
tb	566.53	K	Cheméo Relay (1.0)
tc	830.14	K	Cheméo Relay (1.0)
tf	358.65	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.87	J/mol×K	631.97	Joback Method
cpg	436.10	J/mol×K	667.17	Joback Method
cpg	449.41	J/mol×K	702.37	Joback Method
cpg	461.85	J/mol×K	737.57	Joback Method
cpg	473.46	J/mol×K	772.77	Joback Method
cpg	484.27	J/mol×K	807.97	Joback Method
cpg	494.34	J/mol×K	843.17	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3083883&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point