N,N'-di-n-Butylurea

Other names:	1,3-Dibutylurea
	N,N'-Dibutylurea
	Urea, N,N'-dibutyl-
Inchi:	InChI=1S/C9H20N2O/c1-3-5-7-10-9(12)11-8-6-4-2/h3-8H2,1-2H3,(H2,10,11,12)
InchiKey:	AQSQFWLMFCKKMG-UHFFFAOYSA-N
Formula:	C9H20N2O
SMILES:	CCCCNC(=O)NCCCC
Mol. weight [g/mol]:	172.27
CAS:	1792-17-2

Physical Properties

Property code	Value	Unit	Source
gf	74.76	kJ/mol	Joback Method
hf	-234.73	kJ/mol	Joback Method
hfus	30.86	kJ/mol	Joback Method
hvap	55.25	kJ/mol	Joback Method
log10ws	-2.72		Crippen Method
logp	1.886		Crippen Method
mcvol	159.200	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
tb	559.53	K	Joback Method
tc	738.83	K	Joback Method
tf	346.90 ± 0.30	K	NIST Webbook
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	472.48	J/mol×K	738.83	Joback Method
cpg	412.17	J/mol×K	589.41	Joback Method
cpg	425.43	J/mol×K	619.30	Joback Method
cpg	438.07	J/mol×K	649.18	Joback Method
cpg	450.11	J/mol×K	679.06	Joback Method
cpg	461.58	J/mol×K	708.95	Joback Method

cpg	398.29	J/mol×K	559.53	Joback Method
hfust	14.87	kJ/mol	346.90	NIST Webbook
hfust	14.87	kJ/mol	346.90	NIST Webbook
hfust	14.87	kJ/mol	349.60	NIST Webbook
hfust	11.10	kJ/mol	311.50	NIST Webbook
hsubt	91.90 ± 0.90	kJ/mol	347.50	NIST Webbook
hsubt	91.90 ± 0.90	kJ/mol	347.50	NIST Webbook
hsubt	90.00 ± 1.00	kJ/mol	350.00	NIST Webbook
hvapt	101.10 ± 1.60	kJ/mol	396.00	NIST Webbook
sfust	42.80	J/mol×K	346.90	NIST Webbook
sfust	35.63	J/mol×K	311.50	NIST Webbook
sfust	42.87	J/mol×K	346.90	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1792172&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
hfust: Enthalpy of fusion at a given temperature
hsubt: Enthalpy of sublimation at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
sfust: Entropy of fusion at a given temperature
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume