Urea, 1-butyl-3-methyl-

Other names: 1-Butyl-3-methylurea
Urea, N-butyl-N'-methyl-
Inchi: InChI=1S/C6H14N2O/c1-3-4-5-8-6(9)7-2/h3-5H2,1-2H3,(H2,7,8,9)
InchiKey: SIVFQKCLFRMMSZ-UHFFFAOYSA-N
Formula: C6H14N2O
SMILES: CCCCNC(=O)NC
Mol. weight [g/mol]: 130.19
CAS: 6135-36-0

Physical Properties

Property code	Value	Unit	Source
gf	49.50	kJ/mol	Joback Method
hf	-172.81	kJ/mol	Joback Method
hfus	23.09	kJ/mol	Joback Method
hvap	48.57	kJ/mol	Joback Method
log10ws	-1.47		Crippen Method
logp	0.716		Crippen Method
mcvol	116.930	ml/mol	McGowan Method
pc	3439.94	kPa	Joback Method
tb	490.89	K	Joback Method
tc	675.74	K	Joback Method
tf	312.63	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.83	J/mol×K	490.89	Joback Method
cpg	273.17	J/mol×K	521.70	Joback Method
cpg	283.99	J/mol×K	552.51	Joback Method
cpg	294.32	J/mol×K	583.32	Joback Method
cpg	304.16	J/mol×K	614.12	Joback Method
cpg	313.53	J/mol×K	644.93	Joback Method
cpg	322.45	J/mol×K	675.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6135360&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
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume