

BUTYL CARBAMATE

Other names:	Carbamic acid, butyl ester USAF el-101 USAF fo-1 n-Butyl carbamate o-butyl carbamate
Inchi:	InChI=1S/C5H11NO2/c1-2-3-4-8-5(6)7/h2-4H2,1H3,(H2,6,7)
InchiKey:	SKKTUOZKZKCGTB-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CCCCOC(N)=O
Mol. weight [g/mol]:	117.15

Physical Properties

Property code	Value	Unit	Source
af	0.6122		Cheméo Relay (1.0)
gf	-176.25	kJ/mol	Joback Method
hf	-516.35	kJ/mol	Cheméo Relay (1.0)
hfus	16.69	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Cheméo Relay (1.0)
ie	10.07	eV	Cheméo Relay (1.0)
log10ws	-0.66		Aqueous Solubility Prediction Method
logp	0.882		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
tb	437.41	K	Cheméo Relay (1.0)
tc	619.43	K	Cheméo Relay (1.0)
tf	214.43	K	Cheméo Relay (1.0)
vc	0.375	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	210.55	J/mol×K	462.62	Joback Method
cpg	219.90	J/mol×K	494.70	Joback Method

cpg	228.90	J/mol×K	526.78	Joback Method
cpg	237.55	J/mol×K	558.86	Joback Method
cpg	245.86	J/mol×K	590.94	Joback Method
cpg	253.81	J/mol×K	623.02	Joback Method
cpg	261.42	J/mol×K	655.10	Joback Method
hsubt	94.00 ± 8.00	kJ/mol	304.00	NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C592358&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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
hsubt:	Enthalpy of sublimation at a given temperature
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
vc:	Critical Volume

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