Tybamate

Other names:	Carbamic acid, butyl-, 2-[[(aminocarbonyl)oxy]methyl]-2-methylpentyl ester
	Carbamic acid, butyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate (ester)
	Benvil
	Depran
	Effisax
	Nospan
	Reposan
	Solacen
	Solacin
	Tibamate
	Tibamax
	Tybatran
	W 713
	2-Methyl-2-Propyltrimethylene butylcarbamate carbamate
	n-Butyl-2-methyl-2-propyl-1,3-propanediol dicarbamate
	Carbamic acid, butyl-, ester with 2-(hydroxymethyl)-2-methylpentyl carbamate
	Carbamic acid, butyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate
	Carbamic acid, ester with 2-(hydroxymethyl)-2-methylpentyl butylcarbamate
	Carbamic acid, ester with 2-methyl-2-propyl-1,3-propanediol butylcarbamate
	Idalene
	Tibamato
	1,3-Propanediol, 2-methyl-2-propyl-, butylcarbamate carbamate
	2-(Hydroxymethyl)-2-(methylpentyl) butylcarbamate carbamate
	2-Methyl-2-propyl-1,3-propanediol butylcarbamate carbamate
	N-n-Butyl-2-methyl-2-propyl-1,3-propanediol dicarbamate
	NSC 172126
	Carbamic acid, butyl-, 3-hydroxy-2-methyl-2-propyl carbamate ester
	1,3-Propanediol, 2-methyl-2-propyl-n-butyldicarbamate
Inchi:	InChI=1S/C13H26N2O4/c1-4-6-8-15-12(17)19-10-13(3,7-5-2)9-18-11(14)16/h4-10H2,1-3
InchiKey:	PRBORDFJHHAISJ-UHFFFAOYSA-N
Formula:	C13H26N2O4
SMILES:	CCCCNC(=O)OCC(C)(CCC)COC(N)=O
Mol. weight [g/mol]:	274.36
CAS:	4268-36-4

Physical Properties

Property code	Value	Unit	Source

gf	-250.58	kJ/mol	Joback Method
hf	-722.74	kJ/mol	Joback Method
hfus	37.88	kJ/mol	Joback Method
hvap	78.62	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.414		Crippen Method
mcvol	228.870	ml/mol	McGowan Method
pc	1915.26	kPa	Joback Method
tb	768.89	K	Joback Method
tc	963.74	K	Joback Method
tf	518.93	K	Joback Method
vc	0.865	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	695.83	J/mol×K	768.89	Joback Method
cpg	710.20	J/mol×K	801.37	Joback Method
cpg	723.67	J/mol×K	833.84	Joback Method
cpg	736.26	J/mol×K	866.32	Joback Method
cpg	748.00	J/mol×K	898.79	Joback Method
cpg	758.92	J/mol×K	931.27	Joback Method
cpg	769.02	J/mol×K	963.74	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4268364&Units=SI

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