

# Carbamic acid, (1-methylethyl)-, 2-[[[(aminocarbonyl)oxy]methyl]-2-methylpentyl ester

Other names:  
ester

(1-Methylethyl)carbamic acid 2-(((aminocarbonyl)oxy)methyl)-2-methylpentyl ester

1,3-Propanediol, 2-methyl-2-propyl-, carbamate isopropylcarbamate

2-((carbamoyloxy)methyl)-2-methylpentyl isopropylcarbamate

2-methyl-2-propyl-1,3-propanediol carbamate isopropylcarbamate

Apesan

Arusal

Atonalyt

Brianil

CB 8019

Calenfa

Cap-O-Tran

Caprodat

Carbamic acid, ester with 2-(hydroxymethyl)-2-methylpentylisopropyl carbamate

Carbamic acid, ester with 2-methyl-2-propyl-1,3-propanediol isopropylcarbamate

Carbamic acid, isopropyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate

Carbamic acid, isopropyl-, 2-(hydroxymethyl)-2-methylpentyl ester carbamate

(ester)  
Carisol

Carisoma

Carisoprodac

Carisoprodacum

Carisoprodol

Carlsodol

Carlsoma

Carlsoprol

Carsodal

Carsodol

Coprobate

Diolene

Domarax

Flexal

Flexartal

Flexartel

Flibol E

Isobamate

Isomeprobamate

Isopropyl meprobamate

Isopropylcarbamic acid, ester with 2-(hydroxymethyl)-2-methylpentyl carbamate

Isoprotan

Isoprotane

Isoprothane

Izoprotan  
 Mediquil  
 Meprobamate  
 Meprocon  
 Mioartrina  
 Miolisodal  
 Miolisodol  
 Mioratrina  
 Mioril  
 Mioriodol  
 N-Isopropyl-2-methyl-2-propyl-1,3-propanediol, dicarbamate  
 NCI-C56235  
 Nospasm  
 RELA  
 Relasom  
 Relax  
 SCH 7307  
 Sanoma  
 Skutamil  
 Soma  
 Somadril  
 Somalgit  
 Somanil  
 Stialgin  
 Tonolyt isopropyl meprobamate

**Inchi:** InChI=1S/C12H24N2O4/c1-5-6-12(4,7-17-10(13)15)8-18-11(16)14-9(2)3/h9H,5-8H2,1-4H2  
**InchiKey:** OFZCIYFFPZCNJE-UHFFFAOYSA-N  
**Formula:** C12H24N2O4  
**SMILES:** CCCC(C)(COC(N)=O)COC(=O)NC(C)C  
**Mol. weight [g/mol]:** 260.33  
**CAS:** 78-44-4

## Physical Properties

Property code	Value	Unit	Source
gf	-261.44	kJ/mol	Joback Method
hf	-707.38	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	76.01	kJ/mol	Joback Method
log10ws	-3.02		Crippen Method

logp	2.023		Crippen Method
mcvol	214.780	ml/mol	McGowan Method
pc	2102.27	kPa	Joback Method
rinpol	1855.00		NIST Webbook
rinpol	1906.60		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1850.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1847.00		NIST Webbook
rinpol	1841.00		NIST Webbook
rinpol	1830.00		NIST Webbook
tb	745.57	K	Joback Method
tc	943.87	K	Joback Method
tf	492.66	K	Joback Method
tt	367.75	K	Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between the dynamic and thermodynamic fragilities
vc	0.802	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.09	J/mol×K	745.57	Joback Method
cpg	655.29	J/mol×K	778.62	Joback Method
cpg	668.59	J/mol×K	811.67	Joback Method
cpg	681.02	J/mol×K	844.72	Joback Method
cpg	692.60	J/mol×K	877.77	Joback Method
cpg	703.34	J/mol×K	910.82	Joback Method
cpg	713.26	J/mol×K	943.87	Joback Method

## Sources

- McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>
- NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C78444&Units=SI>
- Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
- Joback Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)
- Thermal behavior and dynamic fragility in amorphous carisoprodol. Correlation between the dynamic and thermodynamic fragilities:** <https://www.doi.org/10.1016/j.tca.2018.03.012>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>tt:</b>	Triple Point Temperature
<b>vc:</b>	Critical Volume

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