Meprobamate

Other names:

1,3-Propanediol, 2-methyl-2-propyl-, 1,3-dicarbamate
1,3-Propanediol, 2-methyl-2-propyl-, dicarbamate
2,2-Di(carbamoyloxymethyl)pentane
2-Methyl-2-n-propyl-1,3-propanediol dicarbamate
2-Methyl-2-propyl-1,3-propanediol dicarbamate
2-Methyl-2-propyltrimethylene carbamate
3P Bamate
Amepromat
Amosene
Anastress
Anathylmon
Anatimon
Andaksin
Andaxin
Aneural
Aneurol
Aneusral
Aneuxal
Aneuxral
Ansiatan
Ansil
Ansiowas
Anural
Anxietil
Anzil
Apascil
Apasil
Appetrol
Appetrol-Sr
Arcoban
Arpon
Artolon
Ataraxine
Atraxin
Auxietil
Ayeramate
Ayermate
Bamd 400
Bamo 400
Biobamat

Biobamate
Brobamate
Calmadin
Calmax
Calmiren
Canquil-400
Cap-O-Tran
Carb-A-Med
Carbamic acid 2-methyl-2-propyltrimethylene ester
Carbaxin
Cirpon
Cirponyl
Coprobate
Crestanil
Cypron
Cyrpon
Dapaz
Deprol
Despasmol
Dicandiol
Diron
Diurnal
Diurnaldiverondormabrol
Diveron
Dormabrol
Ecuanil
Edenal
Enorden
Epicur
Epikur
Equanil
Equanil suspension
Equatrate
Equilium
Equinil
Equitar
Erina
Estasil
Fas-Cile
Fas-Cile 200
Gadexyl
Gagexyl
Harmonin

Hartol
Holbamate
Ipsotian
Kesso-Bamate
Klort
Larten
Lepenil
Lepetown
Letyl
Libiolan
Madiol
Mar-Bate
Margonil
Mendel
Mepamtin
Mepantin
Mepavlon
Mepiosine
Meposed
Mepr
Mepranil
Mepriam
Meprin
Meprindon
Meprobam
Meprobamat
Meprobamat-Petrasch
Meprobamato
Meproban
Meprocompren
Meprocon
Meprocon CMC
Meprodil
Meprodiol
Meprol
Meproleaf
Mepron
Meprosa
Meprosan
Meprosin
Meprospan
Meprotabs
Meprotan

Meproten
Meprotil
Meprovan
Meprovanmeprozine
Meprozine
Meptran
Meptranactylmilprem
Mesmar
Metractyl
Metranquil
Micrainin
Microbamat
Milpath
Milprem
Miltamato
Miltann
Miltaun
Miltown
Miltrate
Miltuan
Miltwon
Misedant
Morbam
Multaun
My-trans
Neo-Tran
Nephentine
Nervonus
Neuramate
Oasil
Optarket
Orlevol
Orolevol
PMB-200
PMB-400
Pan-Tranquil
Pancalma
Panediol
Pankalma
Paxin
Pensive
Perequietil
Perequil

Perquietil
Pertranquil
Pimal
Placidon
Placitate
Prequil
Probamato
Probamyl
Procalmadiol
Procalmadol
Procalmidol
Procarbamide
Promate
Promato
Proquanil
Protran
Quaname
Quanane
Quanil
Quietidon
Quivet
Rastenil
Reostral
Restenil
Restenyl
Restinal
Restinil
Robamate
SK-Bamate
Sadanyl
Scolazil
Sedabamate
Sedanil
Sedanyl
Sedazil
Sedoquil
Sedoselecta
Selene
Seril
Setran
Shalvaton
Solevione anastress
Sowell

Spantran
Stensolo
Tamate
Tensol
Tensonal
Trankvilan
Tranlisant
Tranmep
Tranquil
Tranquilan
Tranquilate
Tranquilax
Tranquiline
Tranquillin
Tranquilsan
Tranquinol
Tranquisan
Trelmar
Urbil
Urbilat
Vio-Bamate
Vistabamate
Wardamate
Wyseals
Zirpon
[2-(carbamoyloxymethyl)-2-methylpentyl] carbamate

Inchi: InChI=1S/C9H18N2O4/c1-3-4-9(2,5-14-7(10)12)6-15-8(11)13/h3-6H2,1-2H3,(H2,10,12)(H

InchiKey: NPPQSCRMBWNHMW-UHFFFAOYSA-N

Formula: C9H18N2O4

SMILES: CCCC(C)(COC(N)=O)COC(N)=O

Mol. weight [g/mol]: 218.25

CAS: 57-53-4

Physical Properties

Property code	Value	Unit	Source
gf	-307.20	kJ/mol	Joback Method
hf	-659.86	kJ/mol	Joback Method
hfus	27.62	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method

log10ws	-1.74		Aqueous Solubility Prediction Method
log10ws	-1.81		Estimated Solubility Method
logp	0.983		Crippen Method
mcvol	172.510	ml/mol	McGowan Method
pc	2899.85	kPa	Joback Method
rinpol	1758.00		NIST Webbook
rinpol	1764.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1790.00		NIST Webbook
rinpol	1822.80		NIST Webbook
rinpol	1784.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	304.55		NIST Webbook
rinpol	1780.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1796.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1785.00		NIST Webbook
rinpol	1830.00		NIST Webbook
rinpol	1826.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	301.69		NIST Webbook
rinpol	1762.00		NIST Webbook
tb	699.73	K	Joback Method
tc	907.45	K	Joback Method
tf	377.82	K	Aqueous Solubility Prediction Method
tf	378.70 ± 0.50	K	NIST Webbook
tf	376.00 ± 1.00	K	NIST Webbook
vc	0.634	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	490.52	J/mol×K	699.73	Joback Method
cpg	502.81	J/mol×K	734.35	Joback Method
cpg	514.32	J/mol×K	768.97	Joback Method
cpg	525.05	J/mol×K	803.59	Joback Method
cpg	535.03	J/mol×K	838.21	Joback Method
cpg	544.26	J/mol×K	872.83	Joback Method
cpg	552.78	J/mol×K	907.45	Joback Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57534&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume