Mebutamate

Other names:	1,3-Propanediol, 2-methyl-2-(1-methylpropyl)-, dicarbamate
	1,3-Propanediol, 2-sec-butyl-2-methyl-, dicarbamate
	Axiten
	Capla
	Carbuten
	Encapla
	Mebutamat
	Mebutina
	Mioartrina
	No-Press
	Preminex
	Sigmafon
	Vallene
	W 583
	2-sec-Butyl-2-methyltrimethylene dicarbamate
	2,2-Dicarbamyloxymethyl-3-methylpentane
	Carbamic acid, 2-sec-butyl-2-methyltrimethylene ester
	Dicamoylmethtane
	Dormate
	Ipotensivo
	MEGA
	2-sec-Butyl-2-methyl-1,3-propanediol dicarbamate
	2-Methyl-2-sec-butyl-1,3-propanediol dicarbamate
	Butatensin
	2-Methyl-2-(1-methylpropyl)-1,3-propanediol dicarbamate
	Prean
	Dicamoylmethane
	NSC 163921
Inchi:	InChI=1S/C10H20N2O4/c1-4-7(2)10(3,5-15-8(11)13)6-16-9(12)14/h7H,4-6H2,1-3H3,(H2
InchiKey:	LEROTMJVBFSIMP-UHFFFAOYSA-N
Formula:	C10H20N2O4
SMILES:	CCC(C)C(C)(COC(N)=O)COC(N)=O
Mol. weight [g/mol]:	232.28
CAS:	64-55-1

Physical Properties

Property code	Value	Unit	Source

gf	-301.22	kJ/mol	Joback Method
hf	-685.78	kJ/mol	Joback Method
hfus	26.69	kJ/mol	Joback Method
hvap	75.76	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	1.229		Crippen Method
mcvol	186.600	ml/mol	McGowan Method
pc	2643.39	kPa	Joback Method
tb	722.17	K	Joback Method
tc	930.73	K	Joback Method
tf	500.72	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.12	J/mol×K	722.17	Joback Method
cpg	556.14	J/mol×K	756.93	Joback Method
cpg	568.31	J/mol×K	791.69	Joback Method
cpg	579.63	J/mol×K	826.45	Joback Method
cpg	590.13	J/mol×K	861.21	Joback Method
cpg	599.82	J/mol×K	895.97	Joback Method
cpg	608.73	J/mol×K	930.73	Joback Method

Sources

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=C64551&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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