1,3-Propanediol, 2-methyl-2-(1-methylpropyl)-, dicarbamate

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

Physical Properties

Property code	Value	Unit	Source

hf	-934.64	kJ/mol	Cheméo Relay (1.0)
hfus	26.69	kJ/mol	Joback Method
hvap	91.84	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-2.66		Cheméo Relay (1.0)
logp	1.229		Crippen Method
mcvol	186.600	ml/mol	McGowan Method
tb	546.37	K	Cheméo Relay (1.0)
tf	336.11	K	Cheméo Relay (1.0)

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C64551&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

cpg: Ideal gas heat capacity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point