

(R)-2,4-DIHYDROXY-N-(3-HYDROXYPROPYL)-3,3-

Other names:

(+)-Panthenol
(R)-2,4-dihydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutanamide
2,4-Dihydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutanamide, (R)-
2,4-Dihydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutyramide, D-(+)-
Alcopan-250
Bepanthen
Bepanthere
Bepantol
Butanamide, 2,4-dihydroxy-N-(3-hydroxypropyl)-3,3-dimethyl-, (2R)-
Butanamide, 2,4-dihydroxy-N-(3-hydroxypropyl)-3,3-dimethyl-, (R)-
Butyramide, 2,4-dihydroxy-N-(3-hydroxypropyl)-3,3-dimethyl-, D-(+)-
Cozyme
D(+)-2,4-Dihydroxy-N-(3-hydroxypropyl)-3,3-dimethylbutyramide
D(+)-Panthenol
D(+)-Pantotheryl alcohol
D-(+)-2,4-Dihydroxy-3,3-dimethyl-N-(3-hydroxypropyl)butyramide
D-P-A Injection
D-Panthenol 50
D-Pantotheryl alcohol
Dexpanthelol
Dexpanthenol
Dextro pantotheryl alcohol
Ilopan
Intrapan
Motilyn
N-Pantoyl-3-propanolamine
NSC 302962
Panadon
Pantenyl
Panthenol, (+)-
Panthoderm
Pantol
Pantothanol
Pantotheryl alcohol
Pantotherylol
Propanolamine, N-pantoyl-
Provitamin B
Provitamin B5
Thenalton
Urupan

Zentic
d-Panthenol
d-Pantothenol

Inchi: InChI=1S/C9H19NO4/c1-9(2,6-12)7(13)8(14)10-4-3-5-11/h7,11-13H,3-6H2,1-2H3,(H,10,
InchiKey: SNPLKNRPJHDVJA-SSDOTTSWSA-N
Formula: C9H19NO4
SMILES: CC(C)(CO)C(O)C(=O)NCCCO
Mol. weight [g/mol]: 205.25
CAS: 81-13-0

Physical Properties

Property code	Value	Unit	Source
gf	-424.69	kJ/mol	Joback Method
hf	-758.92	kJ/mol	Joback Method
hfus	27.09	kJ/mol	Joback Method
hvap	97.16	kJ/mol	Joback Method
log10ws	-0.22		Crippen Method
logp	-1.136		Crippen Method
mcvol	166.830	ml/mol	McGowan Method
pc	3448.03	kPa	Joback Method
rinpol	1807.00		NIST Webbook
tb	782.23	K	Joback Method
tc	962.77	K	Joback Method
tf	463.66	K	Joback Method
vc	0.621	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	520.69	J/molxK	812.32	Joback Method
cpg	529.32	J/molxK	842.41	Joback Method
cpg	537.49	J/molxK	872.50	Joback Method
cpg	545.21	J/molxK	902.59	Joback Method
cpg	552.52	J/molxK	932.68	Joback Method
cpg	511.55	J/molxK	782.23	Joback Method
cpg	559.46	J/molxK	962.77	Joback Method

dvisc	527.2870000	Paxs	293.15	Interaction of D-panthenol with water molecules - Experimental and computational study
dvisc	261.5440000	Paxs	298.15	Interaction of D-panthenol with water molecules - Experimental and computational study
dvisc	125.6730000	Paxs	303.15	Interaction of D-panthenol with water molecules - Experimental and computational study
dvisc	68.4870000	Paxs	308.15	Interaction of D-panthenol with water molecules - Experimental and computational study
dvisc	37.2520000	Paxs	313.15	Interaction of D-panthenol with water molecules - Experimental and computational study

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C81130&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Interaction of D-panthenol with water molecules - Experimental and computational study:	https://www.doi.org/10.1016/j.jct.2017.10.014
Consistent dynamic study of D-Panthenol in aqueous solutions of glycerol at different temperatures:	https://www.doi.org/10.1016/j.jct.2018.07.006
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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