

2-Propanol, 1-[bis(2-hydroxyethyl)amino]-

Other names:	1-(N,N-Bis(2-hydroxyethyl)amino)-2-propanol 1-(N,N-bis(2-hydroxyethyl)amino)propan-2-ol
Inchi:	InChI=1S/C7H17NO3/c1-7(11)6-8(2-4-9)3-5-10/h7,9-11H,2-6H2,1H3
InchiKey:	ZFECCYLNALETDE-UHFFFAOYSA-N
Formula:	C7H17NO3
SMILES:	CC(O)CN(CCO)CCO
Mol. weight [g/mol]:	163.21
CAS:	6712-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-294.06	kJ/mol	Joback Method
hf	-582.25	kJ/mol	Joback Method
hfus	25.65	kJ/mol	Joback Method
hvap	82.87	kJ/mol	Joback Method
log10ws	0.77		Crippen Method
logp	-1.346		Crippen Method
mcvol	137.080	ml/mol	McGowan Method
pc	3867.48	kPa	Joback Method
tb	648.10	K	Joback Method
tc	807.29	K	Joback Method
tf	368.58	K	Joback Method
vc	0.496	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.49	J/molxK	648.10	Joback Method
cpg	393.41	J/molxK	674.63	Joback Method
cpg	401.94	J/molxK	701.16	Joback Method
cpg	410.07	J/molxK	727.69	Joback Method
cpg	417.84	J/molxK	754.23	Joback Method
cpg	425.26	J/molxK	780.76	Joback Method
cpg	432.33	J/molxK	807.29	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	418.20	K	0.08	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6712987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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