

Dipentaerythritol

Other names:	1,3-Propanediol, 2,2'-[oxybis(methylene)]bis[2-(hydroxymethyl)-Bis[petaerythritol] Dipentek 2,2,6,6,-Tetra(hydroxymethyl)-4-oxaheptane-1,7-diol Hercules Tech Di-PE NSC 65881 2,2,6,6-Tetrakis(hydroxymethyl)-4-oxaheptane-1,7-diol 2,2,2',2'-tetrakis(hydroxymethyl)-3,3'-oxydipropan-1-ol
Inchi:	InChI=1S/C10H22O7/c11-1-9(2-12,3-13)7-17-8-10(4-14,5-15)6-16/h11-16H,1-8H2
InchiKey:	TXBCBTDQIULDIA-UHFFFAOYSA-N
Formula:	C10H22O7
SMILES:	OCC(CO)(CO)COCC(CO)(CO)CO
Mol. weight [g/mol]:	254.28
CAS:	126-58-9

Physical Properties

Property code	Value	Unit	Source
chs	-5507.00 ± 7.90	kJ/mol	NIST Webbook
gf	-886.92	kJ/mol	Joback Method
hf	-1312.83	kJ/mol	Joback Method
hfs	-1572.30 ± 7.90	kJ/mol	NIST Webbook
hfus	32.54	kJ/mol	Joback Method
hvap	137.75	kJ/mol	Joback Method
log10ws	1.81		Crippen Method
logp	-3.070		Crippen Method
mcvol	192.850	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	997.24	K	Joback Method
tc	1252.48	K	Joback Method
tf	594.45	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	668.03	J/mol×K	997.24	Joback Method
cpg	678.10	J/mol×K	1039.78	Joback Method
cpg	687.67	J/mol×K	1082.32	Joback Method
cpg	696.86	J/mol×K	1124.86	Joback Method
cpg	705.79	J/mol×K	1167.40	Joback Method
cpg	714.57	J/mol×K	1209.94	Joback Method
cpg	723.33	J/mol×K	1252.48	Joback Method
dvisc	0.0000025	Pa×s	594.45	Joback Method
dvisc	0.0000003	Pa×s	661.58	Joback Method
dvisc	5.7866606e-08	Pa×s	728.71	Joback Method
dvisc	1.4140963e-08	Pa×s	795.85	Joback Method
dvisc	4.3026699e-09	Pa×s	862.98	Joback Method
dvisc	1.5544968e-09	Pa×s	930.11	Joback Method
dvisc	6.4412511e-10	Pa×s	997.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C126589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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

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