

3-Hexyne-2,5-diol, 2,5-dimethyl-

Other names:	2,5-dimethyl-3-hexyne-2,5-diol 2,5-dimethylhexyne-2,5-diol D 43 Dimethylhexynediol Kemitracin-50 Tetramethylbutynediol
Inchi:	InChI=1S/C8H14O2/c1-7(2,9)5-6-8(3,4)10/h9-10H,1-4H3
InchiKey:	IHJUECRFYCQBMW-UHFFFAOYSA-N
Formula:	C8H14O2
SMILES:	CC(C)(O)C#CC(C)(C)O
Mol. weight [g/mol]:	142.20
CAS:	142-30-3

Physical Properties

Property code	Value	Unit	Source
chs	-4776.40 ± 2.40	kJ/mol	NIST Webbook
chs	-4763.20 ± 1.40	kJ/mol	NIST Webbook
gf	-48.68	kJ/mol	Joback Method
hf	-258.11	kJ/mol	Joback Method
hfs	-385.70 ± 1.40	kJ/mol	NIST Webbook
hfs	-386.00 ± 3.30	kJ/mol	NIST Webbook
hfus	12.95	kJ/mol	Joback Method
hsub	106.70 ± 0.90	kJ/mol	NIST Webbook
hvap	82.80 ± 1.00	kJ/mol	NIST Webbook
ie	9.70	eV	NIST Webbook
log10ws	-1.72		Crippen Method
logp	0.532		Crippen Method
mcvol	126.720	ml/mol	McGowan Method
pc	3886.79	kPa	Joback Method
tb	478.65 ± 2.00	K	NIST Webbook
tc	760.19	K	Joback Method
tf	367.65 ± 1.00	K	NIST Webbook
tf	368.00 ± 3.00	K	NIST Webbook
vc	0.462	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.60	J/mol×K	569.34	Joback Method
cpg	323.75	J/mol×K	601.15	Joback Method
cpg	333.27	J/mol×K	632.96	Joback Method
cpg	342.20	J/mol×K	664.76	Joback Method
cpg	350.57	J/mol×K	696.57	Joback Method
cpg	358.44	J/mol×K	728.38	Joback Method
cpg	365.84	J/mol×K	760.19	Joback Method
hvapt	82.80	kJ/mol	298.15	Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	0.90	NIST Webbook
tbrp	470.50 ± 2.50	K	89.30	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

Vaporization Enthalpies of the r,o-Alkanediols by Correlation Gas Chromatography:

<https://www.doi.org/10.1021/je060333x>

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=C142303&Units=SI>

Legend

chs: Standard solid enthalpy of combustion

cpg:	Ideal gas heat capacity
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
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
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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