2,4,7,9-Tetramethyl-5-decyn-4,7-diol

Other names:	2,4,7,9-Tetramethyl-5-decyne-4,7-diol
	5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-
	Surfynol 104
	Surfynol 104A
	Surfynol 104E
	Syrfynol 104
	1,4-Diisobutyl-1,4-dimethylbutynediol
	Surfynol 104BC
	Surfynol 104H
	Surfynol 104PA
	Surfynol TG
	Tetramethyl decynediol
	2,4,7,9-Tetremathyl-5-decyne-4,7-diol
	NSC 5630
	Olfine AK 02
	2,4,7,9-tetramethyldec-5-yne-4,7-diol
Inchi:	InChI=1S/C14H26O2/c1-11(2)9-13(5,15)7-8-14(6,16)10-12(3)4/h11-12,15-16H,9-10H2,1
InchiKey:	LXOFYPKXCSULTL-UHFFFAOYSA-N
Formula:	C14H26O2
SMILES:	CC(C)CC(C)(O)C#CC(C)(O)CC(C)C
Mol. weight [g/mol]:	226.35
CAS:	126-86-3

Physical Properties

Property code	Value	Unit	Source
gf	-3.04	kJ/mol	Joback Method
hf	-392.51	kJ/mol	Joback Method
hfus	21.44	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	2.584		Crippen Method
mcvol	211.260	ml/mol	McGowan Method
pc	2135.43	kPa	Joback Method
rinpol	1407.30		NIST Webbook
rinpol	1407.30		NIST Webbook
tb	705.74	K	Joback Method
tc	892.60	K	Joback Method

tf	450.12	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	613.69	J/mol×K	705.74	Joback Method
cpg	627.85	J/mol×K	736.88	Joback Method
cpg	641.23	J/mol×K	768.03	Joback Method
cpg	653.90	J/mol×K	799.17	Joback Method
cpg	665.89	J/mol×K	830.31	Joback Method
cpg	677.27	J/mol×K	861.45	Joback Method
cpg	688.09	J/mol×K	892.60	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126863&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature

tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume