2,4,7,9-TETRAMETHYL-5-DECYNE-4,7-DIOL

Other names: 1,4-Diisobutyl-1,4-dimethylbutynediol
2,4,7,9-Tetramethyl-5-decyne-4,7-diol
2,4,7,9-Tetremathyl-5-decyne-4,7-diol
2,4,7,9-tetramethyldec-5-yne-4,7-diol
5-Decyne-4,7-diol, 2,4,7,9-tetramethyl-
NSC 5630
Olfine AK 02
Surfynol 104
Surfynol 104A
Surfynol 104BC
Surfynol 104E
Surfynol 104H
Surfynol 104PA
Surfynol TG
Syrfynol 104
Tetramethyl decynediol

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]: 226.36

Physical Properties

Property code	Value	Unit	Source
af	0.7540		Cheméo Relay (1.0)
gf	-3.04	kJ/mol	Joback Method
hf	-373.12	kJ/mol	Cheméo Relay (1.0)
hfus	21.44	kJ/mol	Joback Method
hvap	94.50	kJ/mol	Cheméo Relay (1.0)
ie	9.41	eV	Cheméo Relay (1.0)
log10ws	-3.17		Cheméo Relay (1.0)
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	520.77	K	Cheméo Relay (1.0)

tc	713.47	K	Cheméo Relay (1.0)
tf	320.29	K	Cheméo Relay (1.0)
vc	0.783	m3/kmol	Cheméo Relay (1.0)

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126863&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
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
ie: Ionization energy
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