4,7-Dimethyl-5-decyne-4,7-diol

Other names:	Surfynol 102 5-Decyne-4,7-diol, 4,7-dimethyl- 4,7-Dimethyl-5-decyn-4,7-diol NSC 5625
Inchi:	InChI=1S/C12H22O2/c1-5-7-11(3,13)9-10-12(4,14)8-6-2/h13-14H,5-8H2,1-4H3
InchiKey:	HCKFFIBKYQSDRD-UHFFFAOYSA-N
Formula:	C12H22O2
SMILES:	CCCC(C)(O)C#CC(C)(O)CCC
Mol. weight [g/mol]:	198.30
CAS:	126-87-4

Physical Properties

Property code	Value	Unit	Source
gf	-15.00	kJ/mol	Joback Method
hf	-340.67	kJ/mol	Joback Method
hfus	23.31	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-3.39		Crippen Method
logp	2.092		Crippen Method
mcvol	183.080	ml/mol	McGowan Method
pc	2530.27	kPa	Joback Method
tb	660.86	K	Joback Method
tc	844.42	K	Joback Method
tf	457.58	K	Joback Method
vc	0.685	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	507.33	J/mol×K	660.86	Joback Method
cpg	520.07	J/mol×K	691.45	Joback Method
cpg	532.12	J/mol×K	722.05	Joback Method
cpg	543.52	J/mol×K	752.64	Joback Method
cpg	554.31	J/mol×K	783.23	Joback Method

cpg	564.55	J/mol×K	813.83	Joback Method
cpg	574.28	J/mol×K	844.42	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	399.00 ± 1.00	K	0.40	NIST Webbook

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=C126874&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
tb: Normal Boiling Point Temperature
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume