3,4,4,-Trimethyl-1-pentyn-3-ol

Inchi: InChI=1S/C8H14O/c1-6-8(5,9)7(2,3)4/h1,9H,2-5H3
InchiKey: XXWIEGOAVMLISY-UHFFFAOYSA-N
Formula: C8H14O
SMILES: C#CC(C)(O)C(C)(C)C
Mol. weight [g/mol]: 126.20
CAS: 993-53-3

Physical Properties

Property code	Value	Unit	Source
gf	108.41	kJ/mol	Joback Method
hf	-86.28	kJ/mol	Joback Method
hfus	8.71	kJ/mol	Joback Method
hvap	47.35	kJ/mol	Joback Method
log10ws	-2.10		Crippen Method
logp	1.417		Crippen Method
mcvol	120.850	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
tb	458.28	K	Joback Method
tc	649.75	K	Joback Method
tf	292.55	K	Joback Method
vc	0.443	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	264.21	J/mol×K	458.28	Joback Method
cpg	276.57	J/mol×K	490.19	Joback Method
cpg	288.10	J/mol×K	522.10	Joback Method
cpg	298.86	J/mol×K	554.02	Joback Method
cpg	308.89	J/mol×K	585.93	Joback Method
cpg	318.26	J/mol×K	617.84	Joback Method
cpg	326.99	J/mol×K	649.75	Joback Method

Sources

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=C993533&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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