2-Methyl-3-pentyn-2-ol

Inchi: InChI=1S/C6H10O/c1-4-5-6(2,3)7/h7H,1-3H3
InchiKey: JPKQHUHDYLMRJW-UHFFFAOYSA-N
Formula: C6H10O
SMILES: CC#CC(C)(C)O
Mol. weight [g/mol]: 98.14
CAS: 590-38-5

Physical Properties

Property code	Value	Unit	Source
gf	68.46	kJ/mol	Joback Method
hf	-55.85	kJ/mol	Joback Method
hfus	11.09	kJ/mol	Joback Method
hvap	46.48	kJ/mol	Joback Method
log10ws	-1.50		Crippen Method
logp	0.781		Crippen Method
mcvol	92.670	ml/mol	McGowan Method
pc	4311.22	kPa	Joback Method
tb	434.63	K	Joback Method
tc	629.45	K	Joback Method
tf	326.72	K	Joback Method
vc	0.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.54	J/mol×K	434.63	Joback Method
cpg	190.81	J/mol×K	467.10	Joback Method
cpg	199.57	J/mol×K	499.57	Joback Method
cpg	207.84	J/mol×K	532.04	Joback Method
cpg	215.65	J/mol×K	564.51	Joback Method
cpg	223.01	J/mol×K	596.98	Joback Method
cpg	229.97	J/mol×K	629.45	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=C590385&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume