

3-Pentyn-2-ol

Inchi:	InChI=1S/C5H8O/c1-3-4-5(2)6/h5-6H,1-2H3
InchiKey:	HJFRLXPEVRXBQZ-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	CC#CC(C)O
Mol. weight [g/mol]:	84.12
CAS:	27301-54-8

Physical Properties

Property code	Value	Unit	Source
gf	54.76	kJ/mol	Joback Method
hf	-31.74	kJ/mol	Joback Method
hfus	12.39	kJ/mol	Joback Method
hvap	45.17	kJ/mol	Joback Method
log10ws	-1.09		Crippen Method
logp	0.390		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4835.95	kPa	Joback Method
tb	414.54	K	Joback Method
tc	603.10	K	Joback Method
tf	298.03	K	Joback Method
vc	0.290	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.46	J/molxK	414.54	Joback Method
cpg	149.57	J/molxK	445.97	Joback Method
cpg	156.39	J/molxK	477.39	Joback Method
cpg	162.95	J/molxK	508.82	Joback Method
cpg	169.24	J/molxK	540.25	Joback Method
cpg	175.27	J/molxK	571.67	Joback Method
cpg	181.06	J/molxK	603.10	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=C27301548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
hvac:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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