2-Penten-4-yn-1-ol

Other names: pent-2-en-4-yn-1-ol
Inchi: InChI=1S/C5H6O/c1-2-3-4-5-6/h1,3-4,6H,5H2/b4-3+
InchiKey: TWJDCTNDUKKEMU-ONEGZZNKSA-N
Formula: C5H6O
SMILES: C#CC=CCO
Mol. weight [g/mol]: 82.10
CAS: 5557-88-0

Physical Properties

Property code	Value	Unit	Source
gf	157.69	kJ/mol	Joback Method
hf	110.36	kJ/mol	Joback Method
hfus	15.97	kJ/mol	Joback Method
hvap	43.22	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.168		Crippen Method
mcvol	74.280	ml/mol	McGowan Method
pc	5058.59	kPa	Joback Method
tb	400.26	K	Joback Method
tc	581.84	K	Joback Method
tf	248.82	K	Joback Method
vc	0.277	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	129.44	J/mol×K	400.26	Joback Method
cpg	135.66	J/mol×K	430.52	Joback Method
cpg	141.51	J/mol×K	460.79	Joback Method
cpg	147.02	J/mol×K	491.05	Joback Method
cpg	152.20	J/mol×K	521.31	Joback Method
cpg	157.09	J/mol×K	551.57	Joback Method
cpg	161.70	J/mol×K	581.84	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	341.50 ± 0.50	K	2.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5557880&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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