

4-Pentyn-1-ol

Other names:	1-Pentyn-5-ol pent-4-yn-1-ol
Inchi:	InChI=1S/C5H8O/c1-2-3-4-5-6/h1,6H,3-5H2
InchiKey:	CRWVOXFUXPYTRK-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	C#CCCCO
Mol. weight [g/mol]:	84.12
CAS:	5390-04-5

Physical Properties

Property code	Value	Unit	Source
gf	77.47	kJ/mol	Joback Method
hf	-6.86	kJ/mol	Joback Method
hfus	15.77	kJ/mol	Joback Method
hvap	43.26	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.392		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4704.19	kPa	Joback Method
ripol	1333.00		NIST Webbook
ripol	1333.00		NIST Webbook
tb	427.20	K	NIST Webbook
tb	427.00	K	NIST Webbook
tc	568.78	K	Joback Method
tf	253.90	K	Joback Method
vc	0.296	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	145.02	J/mol×K	396.10	Joback Method
cpg	151.70	J/mol×K	424.88	Joback Method
cpg	158.09	J/mol×K	453.66	Joback Method
cpg	164.20	J/mol×K	482.44	Joback Method

cpg	170.04	J/mol×K	511.22	Joback Method
cpg	175.61	J/mol×K	540.00	Joback Method
cpg	180.94	J/mol×K	568.78	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64462e+01
Coeff. B	-4.34252e+03
Coeff. C	-5.98560e+01
Temperature range (K), min.	328.15
Temperature range (K), max.	450.15

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5390045&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
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

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

pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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