

2-Pentyn-1-ol

Other names:	pent-2-yn-1-ol
Inchi:	InChI=1S/C5H8O/c1-2-3-4-5-6/h6H,2,5H2,1H3
InchiKey:	WLPYSOCRPHITDZ-UHFFFAOYSA-N
Formula:	C5H8O
SMILES:	CCC#CCO
Mol. weight [g/mol]:	84.12
CAS:	6261-22-9

Physical Properties

Property code	Value	Unit	Source
gf	57.20	kJ/mol	Joback Method
hf	-26.46	kJ/mol	Joback Method
hfus	15.92	kJ/mol	Joback Method
hvap	45.55	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.392		Crippen Method
mcvol	78.580	ml/mol	McGowan Method
pc	4782.59	kPa	Joback Method
tb	414.98	K	Joback Method
tc	599.21	K	Joback Method
tf	313.03	K	Joback Method
vc	0.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	142.38	J/molxK	414.98	Joback Method
cpg	149.23	J/molxK	445.68	Joback Method
cpg	155.82	J/molxK	476.39	Joback Method
cpg	162.17	J/molxK	507.09	Joback Method
cpg	168.26	J/molxK	537.80	Joback Method
cpg	174.12	J/molxK	568.50	Joback Method
cpg	179.75	J/molxK	599.21	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	357.70	K	7.60	NIST Webbook
tbrp	334.50 ± 0.50	K	2.00	NIST Webbook
tbrp	334.70	K	2.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.64795e+01
Coeff. B	-4.10284e+03
Coeff. C	-5.16780e+01
Temperature range (K), min.	305.15
Temperature range (K), max.	419.15

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C6261229&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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