

Pentanol, 5-amino-

Other names:	1-Pentanol, 5-amino- 5-Amino-1-pentanol 5-Aminopentanol-1 5-aminopentan-1-ol
Inchi:	InChI=1S/C5H13NO/c6-4-2-1-3-5-7/h7H,1-6H2
InchiKey:	LQGKDMHENBFVRC-UHFFFAOYSA-N
Formula:	C5H13NO
SMILES:	NCCCCCO
Mol. weight [g/mol]:	103.16
CAS:	2508-29-4

Physical Properties

Property code	Value	Unit	Source
gf	-79.15	kJ/mol	Joback Method
hf	-264.97	kJ/mol	Joback Method
hfus	17.99	kJ/mol	Joback Method
hvap	54.04	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	0.108		Crippen Method
mcvol	97.160	ml/mol	McGowan Method
pc	4167.71	kPa	Joback Method
rinpol	988.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	1075.00		NIST Webbook
ripol	1799.00		NIST Webbook
ripol	1799.00		NIST Webbook
tb	494.70	K	NIST Webbook
tb	494.50 ± 0.50	K	NIST Webbook
tc	652.87	K	Joback Method
tf	311.50 ± 0.50	K	NIST Webbook
vc	0.363	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.97	J/mol×K	478.51	Joback Method
cpg	227.91	J/mol×K	507.57	Joback Method
cpg	236.48	J/mol×K	536.63	Joback Method
cpg	244.69	J/mol×K	565.69	Joback Method
cpg	252.56	J/mol×K	594.75	Joback Method
cpg	260.10	J/mol×K	623.81	Joback Method
cpg	267.31	J/mol×K	652.87	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	395.20	K	2.10	NIST Webbook
tbrp	353.00 ± 1.00	K	0.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.60952e+01
Coeff. B	-4.77479e+03
Coeff. C	-7.86630e+01
Temperature range (K), min.	380.72
Temperature range (K), max.	521.44

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=C2508294&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

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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
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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