

1-Nitropentane

Inchi:	InChI=1S/C5H11NO2/c1-2-3-4-5-8-6-7/h2-5H2,1H3
InchiKey:	BVALZCVRLDMXOQ-UHFFFAOYSA-N
Formula:	C5H11NO2
SMILES:	CCCCCON=O
Mol. weight [g/mol]:	117.15
CAS:	628-05-7

Physical Properties

Property code	Value	Unit	Source
af	0.6175		Cheméo Relay (1.0)
hf	-172.74	kJ/mol	Cheméo Relay (1.0)
hvap	39.85	kJ/mol	Cheméo Relay (1.0)
ie	10.14	eV	Cheméo Relay (1.0)
log10ws	-1.73		Cheméo Relay (1.0)
logp	1.875		Crippen Method
mcvol	98.730	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	373.48	K	Cheméo Relay (1.0)
tc	563.00	K	Cheméo Relay (1.0)
tf	219.90	K	Cheméo Relay (1.0)
vc	0.396	m3/kmol	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.49924e+01
Coeff. B	-3.94872e+03
Coeff. C	-6.50680e+01
Temperature range (K), min.	333.60
Temperature range (K), max.	472.95

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?Str2File=C463047

Legend

af:	Acentric Factor
hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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