

Hexane, 1-nitro-

Other names:	1-Nitrohexane Nitrohexane
Inchi:	InChI=1S/C6H13NO2/c1-2-3-4-5-6-7(8)9/h2-6H2,1H3
InchiKey:	FEYJIFXFOHFGCC-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CCCCCC[N+](=O)[O-]
Mol. weight [g/mol]:	131.17
CAS:	646-14-0

Physical Properties

Property code	Value	Unit	Source
gf	35.19	kJ/mol	Joback Method
hf	-177.93	kJ/mol	Joback Method
hfus	22.66	kJ/mol	Joback Method
hvap	45.54	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	1.843		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3149.09	kPa	Joback Method
rinpol	1008.00		NIST Webbook
rinpol	1004.40		NIST Webbook
rinpol	1011.70		NIST Webbook
rinpol	1009.70		NIST Webbook
rinpol	1050.00		NIST Webbook
tb	488.52	K	Joback Method
tc	690.22	K	Joback Method
tf	300.99	K	Joback Method
vc	0.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.19	J/molxK	488.52	Joback Method
cpg	261.93	J/molxK	522.14	Joback Method

cpg	273.10	J/mol×K	555.75	Joback Method
cpg	283.71	J/mol×K	589.37	Joback Method
cpg	293.78	J/mol×K	622.99	Joback Method
cpg	303.32	J/mol×K	656.60	Joback Method
cpg	312.36	J/mol×K	690.22	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.51124e+01
Coeff. B	-4.14267e+03
Coeff. C	-7.08790e+01
Temperature range (K), min.	350.32
Temperature range (K), max.	493.56

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=C646140&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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