

Nonadecanenitrile

Other names:	1-Cyanooctadecane Nonadecanonitrile Octadecyl cyanide n-Nonadecanonitrile
Inchi:	InChI=1S/C19H37N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20/h2-18H2,1H3
InchiKey:	MVDGSHXQMOKTDJ-UHFFFAOYSA-N
Formula:	C19H37N
SMILES:	CCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	279.50
CAS:	28623-46-3

Physical Properties

Property code	Value	Unit	Source
gf	242.28	kJ/mol	Joback Method
hf	-270.61	kJ/mol	Joback Method
hfus	46.47	kJ/mol	Joback Method
hvap	68.37	kJ/mol	Joback Method
log10ws	-7.64		Crippen Method
logp	7.162		Crippen Method
mcvol	279.950	ml/mol	McGowan Method
pc	1063.10	kPa	Joback Method
rinpol	362.50		NIST Webbook
rinpol	2208.00		NIST Webbook
tb	736.20	K	Joback Method
tc	911.93	K	Joback Method
tf	316.15 ± 1.00	K	NIST Webbook
vc	1.125	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	839.00	J/mol×K	736.20	Joback Method
cpg	857.36	J/mol×K	765.49	Joback Method
cpg	874.85	J/mol×K	794.78	Joback Method

cpg	891.52	J/mol×K	824.06	Joback Method
cpg	907.40	J/mol×K	853.35	Joback Method
cpg	922.51	J/mol×K	882.64	Joback Method
cpg	936.89	J/mol×K	911.93	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40930e+01
Coeff. B	-5.11024e+03
Coeff. C	-1.21058e+02
Temperature range (K), min.	491.22
Temperature range (K), max.	702.99

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28623463&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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