Hexanedinitrile

Other names:	1,4-DICYANOBUTANE ADIPIC ACID DINITRILE ADIPONITRILE Adipic acid nitrile Adipic dinitrile Adipodinitrile Adipyldinitrile HEXANEDIOIC ACID DINITRILE NSC 7617 Nitrile adipico Tetramethylene cyanide Tetramethylene dicyanide UN 2205
Inchi:	InChI=1S/C6H8N2/c7-5-3-1-2-4-6-8/h1-4H2
InchiKey:	BTGRAWJCKBQKAO-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	N#CCCCCC#N
Mol. weight [g/mol]:	108.14
CAS:	111-69-3

Physical Properties

Property code	Value	Unit	Source
gf	266.00	kJ/mol	Joback Method
hf	149.00 ± 2.00	kJ/mol	NIST Webbook
hfl	84.90 ± 0.40	kJ/mol	NIST Webbook
hfus	18.03	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hvap	64.00 ± 1.00	kJ/mol	NIST Webbook
hvap	64.10	kJ/mol	NIST Webbook
log10ws	-2.07		Crippen Method
logp	1.594		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
nfpaf	%!d(float64=2)		KDB
nfpah	%!d(float64=4)		KDB
pc	2940.89	kPa	Joback Method
rinpol	1090.00		NIST Webbook

tb	568.20	K	NIST Webbook
tc	748.95	K	Joback Method
tf	287.36	K	Joback Method
vc	0.423	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.08	J/mol×K	644.90	Joback Method
cpg	236.58	J/mol×K	679.58	Joback Method
cpg	242.74	J/mol×K	714.27	Joback Method
cpg	208.40	J/mol×K	540.84	Joback Method
cpg	216.00	J/mol×K	575.53	Joback Method
cpg	223.23	J/mol×K	610.21	Joback Method
cpg	248.56	J/mol×K	748.95	Joback Method
hfust	18.00	kJ/mol	275.00	NIST Webbook
hvapt	58.70	kJ/mol	435.50	NIST Webbook
rhol	975.26	kg/m3	298.15	Compressibility Studies of Some Copper(I), Silver(I), and Tetrabutylammonium Salts in Acetonitrile + Adiponitrile Binary Mixtures

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.62876e+01
Coeff. B	-6.22480e+03
Coeff. C	-3.47660e+01
Temperature range (K), min.	423.82
Temperature range (K), max.	601.89

Information	Value
Property code	pvap

Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.46196e+02
Coeff. B	-1.98500e+04
Coeff. C	-3.33952e+01
Coeff. D	1.59380e-05
Temperature range (K), min.	275.64
Temperature range (K), max.	781.00

Sources

Fusion and solid-to-solid transitions of a homologous series of alkane α,ω-dinitriles:	https://www.doi.org/10.1016/j.jct.2007.03.005
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1418
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Compressibility Studies of Some Copper(I), Silver(I), and Tetrabutylammonium Salts in Acetonitrile + Adiponitrile Binary Mixtures:	https://www.doi.org/10.1021/je900915p
Temperature Dependence of the Relative Static Permittivity of Homologous Series of Liquid 1,n-Dicyanoalkanes N=C (CH2)n C=N, n = 2 to 6:	https://www.doi.org/10.1021/je300958c
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1418
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C111693&Units=SI

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
nfpaf:	NFPA Fire Rating
nfpah:	NFPA Health Rating
pc:	Critical Pressure

pvap:	Vapor pressure
rhol:	Liquid Density
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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