Propanedinitrile

Other names:	CH2(CN)2
	CYANOACETONITRILE
	Dicyanomethane
	Dwumetylosulfotlenku
	MALONIC ACID DINITRILE
	MALONONITRILE
	Malonic dinitrile
	Malonitrile
	Malonodinitrile
	Methane, dicyano-
	Methylene cyanide
	Methylenedinitrile
	NSC 3769
	Nitril kyseliny malonove
	Rcra waste number U149
	UN 2647
	USAF A-4600
	USAF KF-19
Inchi:	InChI=1S/C3H2N2/c4-2-1-3-5/h1H2
InchiKey:	CUONGYYJJVDODC-UHFFFAOYSA-N
Formula:	C3H2N2
SMILES:	N#CCC#N
Mol. weight [g/mol]:	66.06
CAS:	109-77-3

Physical Properties

Property code	Value	Unit	Source
affp	723.00	kJ/mol	NIST Webbook
basg	694.10	kJ/mol	NIST Webbook
chs	-1654.20 ± 0.20	kJ/mol	NIST Webbook
chs	-1653.00 ± 1.00	kJ/mol	NIST Webbook
gf	240.74	kJ/mol	Joback Method
hf	266.30 ± 1.00	kJ/mol	NIST Webbook
hf	266.00 ± 2.00	kJ/mol	NIST Webbook
hfs	187.90 ± 0.20	kJ/mol	NIST Webbook
hfs	186.00 ± 1.00	kJ/mol	NIST Webbook

hfus	10.70	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hsub	78.37 ± 0.96	kJ/mol	NIST Webbook
hsub	80.00	kJ/mol	NIST Webbook
hsub	78.40	kJ/mol	NIST Webbook
hsub	78.20 ± 1.00	kJ/mol	NIST Webbook
hsub	79.10 ± 0.80	kJ/mol	NIST Webbook
hvap	43.23	kJ/mol	Joback Method
ie	12.80 ± 0.10	eV	NIST Webbook
ie	12.88	eV	NIST Webbook
ie	12.70	eV	NIST Webbook
log10ws	-0.81		Crippen Method
logp	0.424		Crippen Method
mcvol	55.890	ml/mol	McGowan Method
pc	4130.29	kPa	Joback Method
rinpol	801.00		NIST Webbook
ss	130.96	J/mol×K	NIST Webbook
tb	491.70	K	NIST Webbook
tb	493.20	K	NIST Webbook
tc	690.33	K	Joback Method
tf	305.00 ± 2.00	K	NIST Webbook
tf	307.60 ± 0.60	K	NIST Webbook
tf	304.65 ± 1.50	K	NIST Webbook
tf	304.80	K	KDB
tf	304.00 ± 3.00	K	NIST Webbook
tt	304.99 ± 0.02	K	NIST Webbook
tt	304.91 ± 0.06	K	NIST Webbook
tt	304.98 ± 0.02	K	NIST Webbook
vc	0.256	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	92.95	J/mol×K	472.20	Joback Method
cpg	96.26	J/mol×K	508.56	Joback Method
cpg	99.42	J/mol×K	544.91	Joback Method
cpg	102.42	J/mol×K	581.27	Joback Method
cpg	105.27	J/mol×K	617.62	Joback Method
cpg	107.98	J/mol×K	653.98	Joback Method
cpg	110.54	J/mol×K	690.33	Joback Method

cps	110.29	J/mol×K	298.15	NIST Webbook
hfust	10.70	kJ/mol	305.00	NIST Webbook
hfust	10.80	kJ/mol	305.00	NIST Webbook
hfust	10.80	kJ/mol	305.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	2.70	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.58259e+01
Coeff. B	-5.23199e+03
Coeff. C	-2.63730e+01
Temperature range (K), min.	363.09
Temperature range (K), max.	523.97

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Liquid-Liquid Equilibria in Binary Mixtures of Water with Malonitrile, Succinonitrile, and Glutaronitrile:	https://www.doi.org/10.1021/je049806v
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109773&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1413
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

affp:	Proton affinity
basg:	Gas basicity
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
rinpol:	Non-polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume