Butanedinitrile

Other names:	1,2-DICYANOETHANE
	1,4-Butanedinitrile
	Deprelin
	Dician
	Dinile
	Disuxyl
	ETHYLENE DICYANIDE
	Ethane, 1,2-dicyano-
	Ethylene cyanide
	Evanex
	NCCH2CH2CN
	NSC 4852
	SUCCINONITRILE
	Succinic acid dinitrile
	Succinic acid nitrile
	Succinic dinitrile
	Succinil
	Succinodinitrile
	Sukcinonitril
	Suxil
	USAF A-9442
	s-Dicyanoethane
	sym-Dicyanoethane
Inchi:	InChI=1S/C4H4N2/c5-3-1-2-4-6/h1-2H2
InchiKey:	IAHFWCOBPZCAEA-UHFFFAOYSA-N
Formula:	C4H4N2
SMILES:	N#CCCC#N
Mol. weight [g/mol]:	80.09
CAS:	110-61-2

Physical Properties

Property code	Value	Unit	Source
chs	-2285.40 ± 0.59	kJ/mol	NIST Webbook
ea	0.02 ± 0.00	eV	NIST Webbook
ea	0.11 ± 0.01	eV	NIST Webbook
gf	249.16	kJ/mol	Joback Method

hf	209.70 ± 0.88	kJ/mol	NIST Webbook
hfs	139.70 ± 0.67	kJ/mol	NIST Webbook
hfus	3.75	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hfus	3.70	kJ/mol	Thermal, solid liquid equilibrium, crystallization, and microstructural studies of organic monotectic alloy: 4,4 -Dibromobiphenyl succinonitrile
hsub	70.00	kJ/mol	NIST Webbook
hvap	45.45	kJ/mol	Joback Method
ie	12.10 ± 0.25	eV	NIST Webbook
log10ws	-1.23		Crippen Method
logp	0.814		Crippen Method
mcvol	69.980	ml/mol	McGowan Method
pc	3664.21	kPa	Joback Method
ss	191.59	J/mol×K	NIST Webbook
tb	539.20	K	NIST Webbook
tc	709.86	K	Joback Method
tf	330.32 ± 0.30	K	NIST Webbook
tf	328.15 ± 1.00	K	NIST Webbook
tf	334.00 ± 1.00	K	NIST Webbook
tf	334.00 ± 1.00	K	NIST Webbook
tf	330.60 ± 0.50	K	NIST Webbook
tf	330.62 ± 0.25	K	NIST Webbook
tf	331.25 ± 0.15	K	NIST Webbook
tf	326.00 ± 4.00	K	NIST Webbook
tf	330.05 ± 0.20	K	NIST Webbook
tf	326.00 ± 3.00	K	NIST Webbook
tf	330.10 ± 0.60	K	NIST Webbook
tt	331.23 ± 0.01	K	NIST Webbook
tt	331.22 ± 0.01	K	NIST Webbook
tt	331.23 ± 0.00	K	NIST Webbook
tt	331.16 ± 0.02	K	NIST Webbook
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	155.23	J/mol×K	709.86	Joback Method

cpg	151.46	J/mol×K	674.06	Joback Method
cpg	147.48	J/mol×K	638.26	Joback Method
cpg	143.28	J/mol×K	602.47	Joback Method
cpg	138.85	J/mol×K	566.67	Joback Method
cpg	134.19	J/mol×K	530.88	Joback Method
cpg	129.29	J/mol×K	495.08	Joback Method
cps	145.60	J/mol×K	298.15	NIST Webbook
hfust	3.75	kJ/mol	330.30	NIST Webbook
hfust	3.70	kJ/mol	329.70	NIST Webbook
hfust	3.70	kJ/mol	334.00	NIST Webbook
hfust	3.70	kJ/mol	331.20	NIST Webbook
hfust	6.20	kJ/mol	233.30	NIST Webbook
hfust	3.70	kJ/mol	177.50	NIST Webbook
hsubt	70.00 ± 0.30	kJ/mol	288.50	NIST Webbook
sfust	11.10	J/mol×K	334.00	NIST Webbook
sfust	11.21	J/mol×K	331.20	NIST Webbook
sfust	26.57	J/mol×K	233.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52708e+01
Coeff. B	-4.82831e+03
Coeff. C	-8.59420e+01
Temperature range (K), min.	408.19
Temperature range (K), max.	572.01

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	4.32550e+01
Coeff. B	-9.16780e+03
Coeff. C	-3.39283e+00
Coeff. D	-1.16457e-06
Temperature range (K), min.	279.15
Temperature range (K), max.	770.00

Sources

Liquid-Liquid Equilibria in Binary Mixtures of Water with Malonitrile, Succinonitrile, and Glutaronitrile:	https://www.doi.org/10.1021/je049806v
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1414
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1414
Thermal, solid liquid equilibrium, crystallization, and microstructural studies of organic monotectic alloy: 4,4 Dibromobiphenyl succinonitrile:	https://www.doi.org/10.1016/j.tca.2009.06.012
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C110612&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
ea:	Electron affinity
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
hsubt:	Enthalpy of sublimation at a given temperature
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume