Pentanedinitrile

Other names:	1,3-DICYANOPROPANE
	1,3-Trimethylenedinitrile
	GLUTARONITRILE
	Glutaric acid dinitrile
	Glutaric dinitrile
	Glutarodinitrile
	TRIMETHYLENE DICYANIDE
Inchi:	InChI=1S/C5H6N2/c6-4-2-1-3-5-7/h1-3H2
InchiKey:	ZTOMUSMDRMJOTH-UHFFFAOYSA-N
Formula:	C5H6N2
SMILES:	N#CCCCC#N
Mol. weight [g/mol]:	94.11
CAS:	544-13-8

Physical Properties

Property code	Value	Unit	Source
gf	257.58	kJ/mol	Joback Method
hf	183.23	kJ/mol	Joback Method
hfus	12.03	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hvap	47.68	kJ/mol	Joback Method
log10ws	-1.65		Crippen Method
logp	1.204		Crippen Method
mcvol	84.070	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
sl	239.45	J/mol×K	NIST Webbook
tb	559.35 ± 3.00	K	NIST Webbook
tb	559.20	K	NIST Webbook
tc	729.38	K	Joback Method
tf	243.60 ± 0.60	K	NIST Webbook
tt	244.21 ± 0.02	K	NIST Webbook
vc	0.367	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.81	J/mol×K	517.96	Joback Method
cpg	174.14	J/mol×K	553.20	Joback Method
cpg	180.15	J/mol×K	588.43	Joback Method
cpg	185.86	J/mol×K	623.67	Joback Method
cpg	191.28	J/mol×K	658.91	Joback Method
cpg	196.41	J/mol×K	694.14	Joback Method
cpg	201.25	J/mol×K	729.38	Joback Method
cpl	186.26	J/mol×K	298.15	NIST Webbook
hfust	12.59	kJ/mol	244.21	NIST Webbook
hfust	12.03	kJ/mol	242.00	NIST Webbook
hfust	12.59	kJ/mol	244.20	NIST Webbook
hfust	12.59	kJ/mol	244.20	NIST Webbook
hvapt	60.10	kJ/mol	462.00	NIST Webbook
hvapt	66.80	kJ/mol	290.00	NIST Webbook
sfust	51.53	J/mol×K	244.21	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60720e+01
Coeff. B	-5.95750e+03
Coeff. C	-3.90620e+01
Temperature range (K), min.	416.49
Temperature range (K), max.	592.71

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	9.90371e+01
Coeff. B	-1.13046e+04
Coeff. C	-1.20138e+01
Coeff. D	5.75911e-06

Temperature range (K), min.	244.21
Temperature range (K), max.	782.00

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544138&Units=SI
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1416
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=1416
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
gf:	Standard Gibbs free energy of formation
hf:	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
pc:	Critical Pressure
pvap:	Vapor pressure
sfust:	Entropy of fusion at a given temperature
sl:	Liquid 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