Pentanedinitrile, 2-methyl-

Other names:	1,3-Dicyanobutane
	1,5-VALERODINITRILE
	1,5-Valerodinitrile, 2-methyl-
	2,4-Dicyanobutane
	2-METHYL PENTANEDINITRILE
	2-Methyl glutarodinitrile
	2-Methylglutaronitrile
	Diacrylonitrile
	Glutaronitrile, 2-methyl-
	METHYLGLUTARONITRILE
	MGN
	«alpha»-Methylglutarodinitrile
	«alpha»-Methylglutaronitrile
	Â«alphaÂ»-Methylglutarodinitrile
	Â«alphaÂ»-Methylglutaronitrile
Inchi:	InChI=1S/C6H8N2/c1-6(5-8)3-2-4-7/h6H,2-3H2,1H3
InchiKey:	FPPLREPCQJZDAQ-UHFFFAOYSA-N
Formula:	C6H8N2
SMILES:	CC(C#N)CCC#N
Mol. weight [g/mol]:	108.14
CAS:	4553-62-2

Physical Properties

Property code	Value	Unit	Source
gf	263.56	kJ/mol	Joback Method
hf	157.31	kJ/mol	Joback Method
hfus	10.79	kJ/mol	Joback Method
hvap	49.52	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.450		Crippen Method
mcvol	98.160	ml/mol	McGowan Method
pc	2966.57	kPa	Joback Method
tb	540.40	K	Joback Method
tc	753.09	K	Joback Method
tf	272.36	K	Joback Method
vc	0.417	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.80	J/mol×K	540.40	Joback Method
cpg	216.64	J/mol×K	575.85	Joback Method
cpg	224.07	J/mol×K	611.30	Joback Method
cpg	231.11	J/mol×K	646.74	Joback Method
cpg	237.77	J/mol×K	682.19	Joback Method
cpg	244.05	J/mol×K	717.64	Joback Method
cpg	249.98	J/mol×K	753.09	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	400.70	K	1.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.78976e+01
Coeff. B	-9.19620e+03
Coeff. C	-7.08910e+01
Temperature range (K), min.	403.97
Temperature range (K), max.	478.05

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
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1419
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4553622&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume