

Decanedinitrile

Other names:	1,8-Dicyanoctane Octamethylene dicyanide Octane-1,8-dicarbonitrile Oktamethylendikyanid Sebacic acid dinitrile sebaconitrile
Inchi:	InChI=1S/C10H16N2/c11-9-7-5-3-1-2-4-6-8-10-12/h1-8H2
InchiKey:	DFJYZCUIKPGCSG-UHFFFAOYSA-N
Formula:	C10H16N2
SMILES:	N#CCCCCCCCCC#N
Mol. weight [g/mol]:	164.25
CAS:	1871-96-1

Physical Properties

Property code	Value	Unit	Source
gf	299.68	kJ/mol	Joback Method
hf	80.03	kJ/mol	Joback Method
hfus	28.17	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hvap	58.81	kJ/mol	Joback Method
log10ws	-3.74		Crippen Method
logp	3.154		Crippen Method
mcvol	154.520	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
tb	472.70	K	NIST Webbook
tc	828.85	K	Joback Method
tf	332.44	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	431.69	J/mol×K	763.35	Joback Method

cpg	440.94	J/mol×K	796.10	Joback Method
cpg	389.33	J/mol×K	632.36	Joback Method
cpg	400.76	J/mol×K	665.11	Joback Method
cpg	411.62	J/mol×K	697.86	Joback Method
cpg	421.93	J/mol×K	730.61	Joback Method
cpg	449.70	J/mol×K	828.85	Joback Method
hfust	28.20	kJ/mol	281.20	NIST Webbook
hvapt	83.70	kJ/mol	323.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1871961&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Fusion and solid-to-solid transitions of a homologous series of alkanes, alkenes, and alkynes:	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

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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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