Octanedinitrile

Other names: 1,6-dicyanohexane
suberonitrile
Inchi: InChI=1S/C8H12N2/c9-7-5-3-1-2-4-6-8-10/h1-6H2
InchiKey: BTNXBLUGMAMSSH-UHFFFAOYSA-N
Formula: C8H12N2
SMILES: N#CCCCCCCC#N
Mol. weight [g/mol]: 136.19
CAS: 629-40-3

Physical Properties

Property code	Value	Unit	Source
gf	282.84	kJ/mol	Joback Method
hf	121.31	kJ/mol	Joback Method
hfus	21.97	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hvap	54.36	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.374		Crippen Method
mcvol	126.340	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
tb	586.60	K	Joback Method
tc	788.48	K	Joback Method
tf	309.90	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	331.47	J/mol×K	721.19	Joback Method
cpg	339.36	J/mol×K	754.84	Joback Method
cpg	295.35	J/mol×K	586.60	Joback Method
cpg	305.10	J/mol×K	620.25	Joback Method
cpg	314.36	J/mol×K	653.89	Joback Method

cpg	323.14	J/mol×K	687.54	Joback Method
cpg	346.82	J/mol×K	788.48	Joback Method
hfust	21.97	kJ/mol	268.90	NIST Webbook
hvapt	77.30	kJ/mol	321.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	458.20	K	2.00	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629403&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Fusion and solid-to-solid transitions of a homologous series of alkane-α,ω-diamines:	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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tbrp:	Boiling point at reduced pressure

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