

Azeleonitrile

Other names:	1,7-dicyanoheptane 1,9-Nonanedinitrile Azelaic dinitrile Nonanedinitrile- azelanitrile azelaonitrile nonanedinitrile
Inchi:	InChI=1S/C9H14N2/c10-8-6-4-2-1-3-5-7-9-11/h1-7H2
InchiKey:	QXOYPGTWWXJFDI-UHFFFAOYSA-N
Formula:	C9H14N2
SMILES:	N#CCCCCCCC#N
Mol. weight [g/mol]:	150.22
CAS:	1675-69-0

Physical Properties

Property code	Value	Unit	Source
gf	291.26	kJ/mol	Joback Method
hf	100.67	kJ/mol	Joback Method
hfus	18.68	kJ/mol	Fusion and solid-to-solid transitions of a homologous series of alkane-a,w-dinitriles
hvap	56.58	kJ/mol	Joback Method
log10ws	-3.32		Crippen Method
logp	2.764		Crippen Method
mcvol	140.430	ml/mol	McGowan Method
pc	2200.01	kPa	Joback Method
tb	609.48	K	Joback Method
tc	808.54	K	Joback Method
tf	321.17	K	Joback Method
vc	0.592	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
---------------	-------	------	-----------------	--------

cpg	341.51	J/mol×K	609.48	Joback Method
cpg	352.16	J/mol×K	642.66	Joback Method
cpg	362.26	J/mol×K	675.83	Joback Method
cpg	371.85	J/mol×K	709.01	Joback Method
cpg	380.94	J/mol×K	742.19	Joback Method
cpg	389.55	J/mol×K	775.36	Joback Method
cpg	397.70	J/mol×K	808.54	Joback Method
hfust	18.68	kJ/mol	251.10	NIST Webbook
hvapt	80.40	kJ/mol	324.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	448.70	K	1.50	NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1675690&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 alkanes, n-alkanes:	https://www.doi.org/10.1016/j.jct.2007.03.005
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

Latest version available from:

<https://www.chemeo.com/cid/59-023-1/Azeleonitrile.pdf>

Generated by Cheméo on 2024-04-26 15:18:33.425134776 +0000 UTC m=+16433962.345712088.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.