

Eicosanenitrile

Other names:	Eicosanonitrile
Inchi:	InChI=1S/C20H39N/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h2-19H2,1
InchiKey:	BYCIKRXQXRFYED-UHFFFAOYSA-N
Formula:	C20H39N
SMILES:	CCCCCCCCCCCCCCCCCCCC#N
Mol. weight [g/mol]:	293.53
CAS:	4616-73-3

Physical Properties

Property code	Value	Unit	Source
gf	250.70	kJ/mol	Joback Method
hf	-291.25	kJ/mol	Joback Method
hfus	49.06	kJ/mol	Joback Method
hvap	70.59	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	7.552		Crippen Method
mcvol	294.040	ml/mol	McGowan Method
pc	999.54	kPa	Joback Method
tb	759.08	K	Joback Method
tc	936.41	K	Joback Method
tf	323.15 ± 2.00	K	NIST Webbook
vc	1.181	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	898.48	J/mol×K	759.08	Joback Method
cpg	917.27	J/mol×K	788.63	Joback Method
cpg	935.16	J/mol×K	818.19	Joback Method
cpg	952.20	J/mol×K	847.74	Joback Method
cpg	968.41	J/mol×K	877.30	Joback Method
cpg	983.83	J/mol×K	906.85	Joback Method
cpg	998.49	J/mol×K	936.41	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.40579e+01
Coeff. B	-5.18352e+03
Coeff. C	-1.24394e+02
Temperature range (K), min.	500.82
Temperature range (K), max.	717.04

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4616733&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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