

Neryl nitrile

Inchi:	InChI=1S/C10H15N/c1-9(2)5-4-6-10(3)7-8-11/h5,7H,4,6H2,1-3H3/b10-7-
InchiKey:	HLCSDJLATUNSSI-YFHOEESVSA-N
Formula:	C10H15N
SMILES:	CC(C)=CCCC(C)=CC#N
Mol. weight [g/mol]:	149.23

Physical Properties

Property code	Value	Unit	Source
gf	309.84	kJ/mol	Joback Method
hf	130.01	kJ/mol	Joback Method
hfus	20.95	kJ/mol	Joback Method
hvap	48.41	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.203		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1227.00		NIST Webbook
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tb	538.36	K	Joback Method
tc	742.94	K	Joback Method
tf	229.37	K	Joback Method
vc	0.584	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.39	J/mol×K	538.36	Joback Method
cpg	335.31	J/mol×K	572.46	Joback Method
cpg	347.49	J/mol×K	606.55	Joback Method
cpg	358.97	J/mol×K	640.65	Joback Method
cpg	369.81	J/mol×K	674.75	Joback Method
cpg	380.06	J/mol×K	708.84	Joback Method
cpg	389.75	J/mol×K	742.94	Joback Method

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=U108905&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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