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)=CCC/C(C)=C\C#N
Mol. weight [g/mol]: 149.24

Physical Properties

Property code	Value	Unit	Source
hf	83.55	kJ/mol	Cheméo Relay (1.0)
hfus	20.95	kJ/mol	Joback Method
hvap	60.92	kJ/mol	Cheméo Relay (1.0)
log10ws	-3.33		Cheméo Relay (1.0)
logp	3.203		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1227.00		NIST Webbook
tb	498.16	K	Cheméo Relay (1.0)
tf	224.37	K	Cheméo Relay (1.0)

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U108905&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point