

(E)-1-Nitroheptadec-1-ene

Inchi:	InChI=1S/C17H33NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18(19)20/h16-17H,2
InchiKey:	ZQRFZDQJAIBDKX-WUKNDPDISA-N
Formula:	C17H33NO2
SMILES:	CCCCCCCCCCCCCCC=C[N+](=O)[O-]
Mol. weight [g/mol]:	283.45

Physical Properties

Property code	Value	Unit	Source
gf	208.03	kJ/mol	Joback Method
hf	-287.75	kJ/mol	Joback Method
hfus	51.35	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-7.37		Crippen Method
logp	6.258		Crippen Method
mvol	263.510	ml/mol	McGowan Method
pc	1288.36	kPa	Joback Method
rinpol	2222.00		NIST Webbook
rinpol	2222.00		NIST Webbook
tb	744.36	K	Joback Method
tc	931.88	K	Joback Method
tf	419.88	K	Joback Method
vc	1.050	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	790.02	J/mol×K	744.36	Joback Method
cpg	807.82	J/mol×K	775.61	Joback Method
cpg	824.73	J/mol×K	806.87	Joback Method
cpg	840.78	J/mol×K	838.12	Joback Method
cpg	856.02	J/mol×K	869.38	Joback Method
cpg	870.50	J/mol×K	900.63	Joback Method
cpg	884.27	J/mol×K	931.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R518646&Units=SI

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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