

(E)-1-Nitropentadec-1-ene

Inchi:	InChI=1S/C15H29NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h14-15H,2-13H2
InchiKey:	VXUKZOXLZJQOHU-CCEZHUSRSA-N
Formula:	C15H29NO2
SMILES:	CCCCCCCCCCCCC=C[N+](=O)[O-]
Mol. weight [g/mol]:	255.40

Physical Properties

Property code	Value	Unit	Source
gf	191.19	kJ/mol	Joback Method
hf	-246.47	kJ/mol	Joback Method
hfus	46.17	kJ/mol	Joback Method
hvap	65.53	kJ/mol	Joback Method
log10ws	-6.53		Crippen Method
logp	5.478		Crippen Method
mcvol	235.330	ml/mol	McGowan Method
pc	1486.14	kPa	Joback Method
rinsol	2019.00		NIST Webbook
tb	698.60	K	Joback Method
tc	887.46	K	Joback Method
tf	397.34	K	Joback Method
vc	0.938	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.29	J/mol×K	698.60	Joback Method
cpg	693.40	J/mol×K	730.08	Joback Method
cpg	709.64	J/mol×K	761.55	Joback Method
cpg	725.05	J/mol×K	793.03	Joback Method
cpg	739.68	J/mol×K	824.51	Joback Method
cpg	753.56	J/mol×K	855.99	Joback Method
cpg	766.74	J/mol×K	887.46	Joback Method

Sources

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=R518651&Units=SI
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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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