

1-Nitrotridec-1-ene

Inchi:	InChI=1S/C13H25NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14(15)16/h12-13H,2-11H2,1H3/b
InchiKey:	FQVYCQNAJYLLDY-OUKQBFOZSA-N
Formula:	C13H25NO2
SMILES:	CCCCCCCCCCC=C[N+](=O)[O-]
Mol. weight [g/mol]:	227.34

Physical Properties

Property code	Value	Unit	Source
gf	174.35	kJ/mol	Joback Method
hf	-205.19	kJ/mol	Joback Method
hfus	40.99	kJ/mol	Joback Method
hvap	61.08	kJ/mol	Joback Method
log10ws	-5.70		Crippen Method
logp	4.698		Crippen Method
mvol	207.150	ml/mol	McGowan Method
pc	1733.22	kPa	Joback Method
rinpol	1808.00		NIST Webbook
tb	652.84	K	Joback Method
tc	844.83	K	Joback Method
tf	374.80	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	567.28	J/molxK	652.84	Joback Method
cpg	583.60	J/molxK	684.84	Joback Method
cpg	599.07	J/molxK	716.84	Joback Method
cpg	613.73	J/molxK	748.83	Joback Method
cpg	627.64	J/molxK	780.83	Joback Method
cpg	640.82	J/molxK	812.83	Joback Method
cpg	653.32	J/molxK	844.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R518631&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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	McGowan's characteristic volume
pc:	Critical Pressure
r inpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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