1-Nitrohexadec-1-ene

Inchi: InChI=1S/C16H31NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17(18)19/h15-16H,2-14
InchiKey: RONABZRHJOUJTH-FOCLMDBBSA-N
Formula: C16H31NO2
SMILES: CCCCCCCCCCCCCCC=C[N+](=O)[O-]
Mol. weight [g/mol]: 269.42

Physical Properties

Property code	Value	Unit	Source
gf	199.61	kJ/mol	Joback Method
hf	-267.11	kJ/mol	Joback Method
hfus	48.76	kJ/mol	Joback Method
hvap	67.76	kJ/mol	Joback Method
log10ws	-6.95		Crippen Method
logp	5.868		Crippen Method
mcvol	249.420	ml/mol	McGowan Method
pc	1381.96	kPa	Joback Method
rinpol	2092.00		NIST Webbook
rinpol	2092.00		NIST Webbook
tb	721.48	K	Joback Method
tc	909.43	K	Joback Method
tf	408.61	K	Joback Method
vc	0.994	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	732.60	J/mol×K	721.48	Joback Method
cpg	750.06	J/mol×K	752.80	Joback Method
cpg	766.65	J/mol×K	784.13	Joback Method
cpg	782.38	J/mol×K	815.45	Joback Method
cpg	797.32	J/mol×K	846.78	Joback Method
cpg	811.51	J/mol×K	878.10	Joback Method
cpg	825.00	J/mol×K	909.43	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=R518611&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume