Nitropentadecane

Inchi: InChI=1S/C15H31NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16(17)18/h2-15H2,1H3
InchiKey: GQUKFPOTLYZVDB-UHFFFAOYSA-N
Formula: C15H31NO2
SMILES: CCCCCCCCCCCCCCC[N+](=O)[O-]
Mol. weight [g/mol]: 257.41

Physical Properties

Property code	Value	Unit	Source
gf	110.97	kJ/mol	Joback Method
hf	-363.69	kJ/mol	Joback Method
hfus	45.97	kJ/mol	Joback Method
hvap	65.58	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	5.354		Crippen Method
mcvol	239.630	ml/mol	McGowan Method
pc	1428.30	kPa	Joback Method
rinpol	1976.00		NIST Webbook
tb	694.44	K	Joback Method
tc	877.73	K	Joback Method
tf	402.42	K	Joback Method
vc	0.958	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	698.79	J/mol×K	694.44	Joback Method
cpg	716.36	J/mol×K	724.99	Joback Method
cpg	733.06	J/mol×K	755.54	Joback Method
cpg	748.94	J/mol×K	786.09	Joback Method
cpg	764.01	J/mol×K	816.64	Joback Method
cpg	778.31	J/mol×K	847.18	Joback Method
cpg	791.88	J/mol×K	877.73	Joback Method

Sources

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=R518686&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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