1-Nitro decane

Inchi: InChI=1S/C10H21NO2/c1-2-3-4-5-6-7-8-9-10-11(12)13/h2-10H2,1H3
InchiKey: GOLOHAZKJYGKKQ-UHFFFAOYSA-N
Formula: C10H21NO2
SMILES: CCCCCCCCCC[N+](=O)[O-]
Mol. weight [g/mol]: 187.28
CAS: 4609-87-4

Physical Properties

Property code	Value	Unit	Source
gf	68.87	kJ/mol	Joback Method
hf	-260.49	kJ/mol	Joback Method
hfus	33.02	kJ/mol	Joback Method
hvap	54.44	kJ/mol	Joback Method
log10ws	-4.09		Crippen Method
logp	3.404		Crippen Method
mcvol	169.180	ml/mol	McGowan Method
pc	2131.49	kPa	Joback Method
tb	580.04	K	Joback Method
tc	771.35	K	Joback Method
tf	346.07	K	Joback Method
vc	0.677	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.68	J/mol×K	580.04	Joback Method
cpg	448.85	J/mol×K	611.92	Joback Method
cpg	463.27	J/mol×K	643.81	Joback Method
cpg	476.98	J/mol×K	675.69	Joback Method
cpg	490.00	J/mol×K	707.58	Joback Method
cpg	502.35	J/mol×K	739.46	Joback Method
cpg	514.06	J/mol×K	771.35	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4609874&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume