1-Nitro octane

Inchi: InChI=1S/C8H17NO2/c1-2-3-4-5-6-7-8-9(10)11/h2-8H2,1H3
InchiKey: KLGHUFNKRIWCDQ-UHFFFAOYSA-N
Formula: C8H17NO2
SMILES: CCCCCCCC[N+](=O)[O-]
Mol. weight [g/mol]: 159.23

Physical Properties

Property code	Value	Unit	Source
gf	52.03	kJ/mol	Joback Method
hf	-219.21	kJ/mol	Joback Method
hfus	27.84	kJ/mol	Joback Method
hvap	49.99	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	2.624		Crippen Method
mcvol	141.000	ml/mol	McGowan Method
pc	2566.29	kPa	Joback Method
tb	534.28	K	Joback Method
tc	730.58	K	Joback Method
tf	323.53	K	Joback Method
vc	0.566	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	338.30	J/mol×K	534.28	Joback Method
cpg	351.98	J/mol×K	567.00	Joback Method
cpg	365.00	J/mol×K	599.71	Joback Method
cpg	377.36	J/mol×K	632.43	Joback Method
cpg	389.10	J/mol×K	665.15	Joback Method
cpg	400.23	J/mol×K	697.86	Joback Method
cpg	410.78	J/mol×K	730.58	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000995&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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