

Hexane, 2-nitro-

Inchi:	InChI=1S/C6H13NO2/c1-3-4-5-6(2)7(8)9/h6H,3-5H2,1-2H3
InchiKey:	KNGSAYHEXMAZMM-UHFFFAOYSA-N
Formula:	C6H13NO2
SMILES:	CCCCC(C)[N+](=O)[O-]
Mol. weight [g/mol]:	131.17
CAS:	14255-44-8

Physical Properties

Property code	Value	Unit	Source
gf	32.75	kJ/mol	Joback Method
hf	-183.21	kJ/mol	Joback Method
hfus	19.13	kJ/mol	Joback Method
hvap	45.15	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	1.842		Crippen Method
mcvol	112.820	ml/mol	McGowan Method
pc	3177.55	kPa	Joback Method
tb	488.08	K	Joback Method
tc	694.38	K	Joback Method
tf	285.99	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	250.42	J/molxK	488.08	Joback Method
cpg	262.51	J/molxK	522.46	Joback Method
cpg	273.99	J/molxK	556.85	Joback Method
cpg	284.88	J/molxK	591.23	Joback Method
cpg	295.19	J/molxK	625.61	Joback Method
cpg	304.95	J/molxK	660.00	Joback Method
cpg	314.17	J/molxK	694.38	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C14255448&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
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

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