Formamide, N-octyl-

Other names: N-Octylformamide
Inchi: InChI=1S/C9H19NO/c1-2-3-4-5-6-7-8-10-9-11/h9H,2-8H2,1H3,(H,10,11)
InchiKey: ZBWPKQRQZDZVSF-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CCCCCCCCNC=O
Mol. weight [g/mol]: 157.25
CAS: 6282-06-0

Physical Properties

Property code	Value	Unit	Source
gf	14.77	kJ/mol	Joback Method
hf	-261.20	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	48.78	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.093		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1505.00		NIST Webbook
rinpol	1505.00		NIST Webbook
tb	504.15	K	Joback Method
tc	677.07	K	Joback Method
tf	285.85	K	Joback Method
vc	0.592	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.83	J/mol×K	504.15	Joback Method
cpg	361.30	J/mol×K	532.97	Joback Method
cpg	374.21	J/mol×K	561.79	Joback Method
cpg	386.56	J/mol×K	590.61	Joback Method
cpg	398.38	J/mol×K	619.43	Joback Method
cpg	409.68	J/mol×K	648.25	Joback Method

cpg	420.47	J/mol×K	677.07	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6282060&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume