Acetamide, N-acetyl-N-heptyl-

Other names: N-Heptyldiacetamide
N-(n-Heptyl)diacetamide
Inchi: InChI=1S/C11H21NO2/c1-4-5-6-7-8-9-12(10(2)13)11(3)14/h4-9H2,1-3H3
InchiKey: PYTBJZCFBMBBGG-UHFFFAOYSA-N
Formula: C11H21NO2
SMILES: CCCCCCCN(C(C)=O)C(C)=O
Mol. weight [g/mol]: 199.29

Physical Properties

Property code	Value	Unit	Source
gf	-105.32	kJ/mol	Joback Method
hf	-428.00	kJ/mol	Joback Method
hfus	30.46	kJ/mol	Joback Method
hvap	55.61	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.352		Crippen Method
mcvol	178.970	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1519.00		NIST Webbook
tb	571.26	K	Joback Method
tc	749.59	K	Joback Method
tf	346.06	K	Joback Method
vc	0.681	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	448.74	J/mol×K	571.26	Joback Method
cpg	463.55	J/mol×K	600.98	Joback Method
cpg	477.66	J/mol×K	630.70	Joback Method
cpg	491.08	J/mol×K	660.42	Joback Method
cpg	503.84	J/mol×K	690.15	Joback Method
cpg	515.96	J/mol×K	719.87	Joback Method
cpg	527.47	J/mol×K	749.59	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373410&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