2-Acetylaminoheptane

Other names:	Acetamide, N-(1-methylhexyl)-
Inchi:	InChI=1S/C9H19NO/c1-4-5-6-7-8(2)10-9(3)11/h8H,4-7H2,1-3H3,(H,10,11)
InchiKey:	XNHVITOEQJZLQB-UHFFFAOYSA-N
Formula:	C9H19NO
SMILES:	CCCCCC(C)NC(C)=O
Mol. weight [g/mol]:	157.25
CAS:	67282-69-3

Physical Properties

Property code	Value	Unit	Source
gf	-17.07	kJ/mol	Joback Method
hf	-293.48	kJ/mol	Joback Method
hfus	22.24	kJ/mol	Joback Method
hvap	48.42	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.091		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1269.00		NIST Webbook
tb	508.92	K	Joback Method
tc	689.58	K	Joback Method
tf	278.78	K	Joback Method
vc	0.575	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.35	J/mol×K	508.92	Joback Method
cpg	361.50	J/mol×K	539.03	Joback Method
cpg	375.03	J/mol×K	569.14	Joback Method
cpg	387.95	J/mol×K	599.25	Joback Method
cpg	400.29	J/mol×K	629.36	Joback Method
cpg	412.05	J/mol×K	659.47	Joback Method
cpg	423.26	J/mol×K	689.58	Joback Method

Sources

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=C67282693&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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