Propanamide, N-hexyl-2-methyl

Inchi: InChI=1S/C10H21NO/c1-4-5-6-7-8-11-10(12)9(2)3/h9H,4-8H2,1-3H3,(H,11,12)
InchiKey: JCQNCGYMFKRRII-UHFFFAOYSA-N
Formula: C10H21NO
SMILES: CCCCCCNC(=O)C(C)C
Mol. weight [g/mol]: 171.28

Physical Properties

Property code	Value	Unit	Source
gf	-8.65	kJ/mol	Joback Method
hf	-314.12	kJ/mol	Joback Method
hfus	24.83	kJ/mol	Joback Method
hvap	50.65	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	2.339		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1352.00		NIST Webbook
tb	531.80	K	Joback Method
tc	710.71	K	Joback Method
tf	290.05	K	Joback Method
vc	0.630	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.18	J/mol×K	531.80	Joback Method
cpg	409.10	J/mol×K	561.62	Joback Method
cpg	423.37	J/mol×K	591.44	Joback Method
cpg	436.99	J/mol×K	621.25	Joback Method
cpg	450.00	J/mol×K	651.07	Joback Method
cpg	462.39	J/mol×K	680.89	Joback Method
cpg	474.20	J/mol×K	710.71	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R50917&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

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