Pentanamide, N-isobutyl

Inchi: InChI=1S/C9H19NO/c1-4-5-6-9(11)10-7-8(2)3/h8H,4-7H2,1-3H3,(H,10,11)
InchiKey: LTGAVKFWROZLPO-UHFFFAOYSA-N
Formula: C9H19NO
SMILES: CCCCC(=O)NCC(C)C
Mol. weight [g/mol]: 157.25

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	-2.31		Crippen Method
logp	1.949		Crippen Method
mcvol	149.220	ml/mol	McGowan Method
pc	2505.01	kPa	Joback Method
rinpol	1281.00		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

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=R50789&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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