Pentanamide, N-isopropyl

Inchi: InChI=1S/C8H17NO/c1-4-5-6-8(10)9-7(2)3/h7H,4-6H2,1-3H3,(H,9,10)
InchiKey: VZEVDNWVJCJQBA-UHFFFAOYSA-N
Formula: C8H17NO
SMILES: CCCCC(=O)NC(C)C
Mol. weight [g/mol]: 143.23

Physical Properties

Property code	Value	Unit	Source
gf	-25.49	kJ/mol	Joback Method
hf	-272.84	kJ/mol	Joback Method
hfus	19.65	kJ/mol	Joback Method
hvap	46.20	kJ/mol	Joback Method
log10ws	-2.25		Crippen Method
logp	1.701		Crippen Method
mcvol	135.130	ml/mol	McGowan Method
pc	2764.26	kPa	Joback Method
rinpol	1152.00		NIST Webbook
tb	486.04	K	Joback Method
tc	668.51	K	Joback Method
tf	267.51	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	302.39	J/mol×K	486.04	Joback Method
cpg	315.67	J/mol×K	516.45	Joback Method
cpg	328.36	J/mol×K	546.86	Joback Method
cpg	340.49	J/mol×K	577.28	Joback Method
cpg	352.07	J/mol×K	607.69	Joback Method
cpg	363.11	J/mol×K	638.10	Joback Method
cpg	373.63	J/mol×K	668.51	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=R50793&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