Propanamide, N-ethyl-2-methyl

Inchi: InChI=1S/C6H13NO/c1-4-7-6(8)5(2)3/h5H,4H2,1-3H3,(H,7,8)
InchiKey: WQLQCNJDXCGKIL-UHFFFAOYSA-N
Formula: C6H13NO
SMILES: CCNC(=O)C(C)C
Mol. weight [g/mol]: 115.17

Physical Properties

Property code	Value	Unit	Source
gf	-42.33	kJ/mol	Joback Method
hf	-231.56	kJ/mol	Joback Method
hfus	14.47	kJ/mol	Joback Method
hvap	41.74	kJ/mol	Joback Method
log10ws	-1.06		Crippen Method
logp	0.778		Crippen Method
mcvol	106.950	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	1002.00		NIST Webbook
tb	440.28	K	Joback Method
tc	626.32	K	Joback Method
tf	244.97	K	Joback Method
vc	0.406	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	218.52	J/mol×K	440.28	Joback Method
cpg	229.69	J/mol×K	471.29	Joback Method
cpg	240.37	J/mol×K	502.29	Joback Method
cpg	250.59	J/mol×K	533.30	Joback Method
cpg	260.35	J/mol×K	564.30	Joback Method
cpg	269.67	J/mol×K	595.31	Joback Method
cpg	278.54	J/mol×K	626.32	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=R50896&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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