N-propyl-butyramide

Other names:	Butanamide, N-propyl- Butyramide, N-propyl- N-n-propyl-butyramide
Inchi:	InChI=1S/C7H15NO/c1-3-5-7(9)8-6-4-2/h3-6H2,1-2H3,(H,8,9)
InchiKey:	TUDFZSGUEDLTJC-UHFFFAOYSA-N
Formula:	C7H15NO
SMILES:	CCCNC(=O)CCC
Mol. weight [g/mol]:	129.20
CAS:	5129-73-7

Physical Properties

Property code	Value	Unit	Source
gf	-31.47	kJ/mol	Joback Method
hf	-246.92	kJ/mol	Joback Method
hfus	20.58	kJ/mol	Joback Method
hvap	44.36	kJ/mol	Joback Method
log10ws	-1.72		Crippen Method
logp	1.313		Crippen Method
mcvol	121.040	ml/mol	McGowan Method
pc	3038.96	kPa	Joback Method
rinpol	1127.00		NIST Webbook
tb	463.60	K	Joback Method
tc	643.92	K	Joback Method
tf	271.24	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	259.27	J/mol×K	463.60	Joback Method
cpg	271.21	J/mol×K	493.65	Joback Method
cpg	282.64	J/mol×K	523.71	Joback Method
cpg	293.59	J/mol×K	553.76	Joback Method
cpg	304.06	J/mol×K	583.82	Joback Method

cpg	314.06	J/mol×K	613.87	Joback Method
cpg	323.61	J/mol×K	643.92	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5129737&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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