Propanamide, 2-methyl-N-ethyl-N-butyl-

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

Physical Properties

Property code	Value	Unit	Source
gf	12.74	kJ/mol	Joback Method
hf	-300.06	kJ/mol	Joback Method
hfus	22.75	kJ/mol	Joback Method
hvap	46.26	kJ/mol	Joback Method
log10ws	-2.11		Crippen Method
logp	2.291		Crippen Method
mcvol	163.310	ml/mol	McGowan Method
pc	2248.26	kPa	Joback Method
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
tb	494.07	K	Joback Method
tc	668.70	K	Joback Method
tf	269.86	K	Joback Method
vc	0.614	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.04	J/mol×K	494.07	Joback Method
cpg	391.55	J/mol×K	523.17	Joback Method
cpg	406.38	J/mol×K	552.28	Joback Method
cpg	420.55	J/mol×K	581.38	Joback Method
cpg	434.07	J/mol×K	610.49	Joback Method
cpg	446.96	J/mol×K	639.59	Joback Method
cpg	459.25	J/mol×K	668.70	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=U415341&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