Propanamide, 2-methyl-N-ethyl-N-3-methylbutyl-

Inchi: InChI=1S/C11H23NO/c1-6-12(8-7-9(2)3)11(13)10(4)5/h9-10H,6-8H2,1-5H3
InchiKey: OPXTZEFDZYQGJV-UHFFFAOYSA-N
Formula: C11H23NO
SMILES: CCN(CCC(C)C)C(=O)C(C)C
Mol. weight [g/mol]: 185.31

Physical Properties

Property code	Value	Unit	Source
gf	18.72	kJ/mol	Joback Method
hf	-325.98	kJ/mol	Joback Method
hfus	21.82	kJ/mol	Joback Method
hvap	48.09	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.537		Crippen Method
mcvol	177.400	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1536.00		NIST Webbook
rinpol	1536.00		NIST Webbook
tb	516.51	K	Joback Method
tc	693.12	K	Joback Method
tf	266.13	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.80	J/mol×K	516.51	Joback Method
cpg	440.40	J/mol×K	545.94	Joback Method
cpg	456.26	J/mol×K	575.38	Joback Method
cpg	471.38	J/mol×K	604.81	Joback Method
cpg	485.79	J/mol×K	634.25	Joback Method
cpg	499.52	J/mol×K	663.68	Joback Method
cpg	512.59	J/mol×K	693.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415342&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