Propanamide, N,N-dibutyl-2,2-dimethyl-

Inchi: InChI=1S/C13H27NO/c1-6-8-10-14(11-9-7-2)12(15)13(3,4)5/h6-11H2,1-5H3
InchiKey: BLSDBULMVZFPPN-UHFFFAOYSA-N
Formula: C13H27NO
SMILES: CCCCN(CCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 213.36

Physical Properties

Property code	Value	Unit	Source
gf	43.28	kJ/mol	Joback Method
hf	-365.45	kJ/mol	Joback Method
hfus	26.63	kJ/mol	Joback Method
hvap	52.03	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.461		Crippen Method
mcvol	205.580	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1451.00		NIST Webbook
tb	559.92	K	Joback Method
tc	736.12	K	Joback Method
tf	321.09	K	Joback Method
vc	0.776	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.32	J/mol×K	559.92	Joback Method
cpg	544.28	J/mol×K	589.29	Joback Method
cpg	561.34	J/mol×K	618.65	Joback Method
cpg	577.54	J/mol×K	648.02	Joback Method
cpg	592.93	J/mol×K	677.39	Joback Method
cpg	607.53	J/mol×K	706.75	Joback Method
cpg	621.38	J/mol×K	736.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308124&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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