Propanamide, N,N-dinonyl-2,2-dimethyl-

Inchi: InChI=1S/C23H47NO/c1-6-8-10-12-14-16-18-20-24(22(25)23(3,4)5)21-19-17-15-13-11-9
InchiKey: AFOUBMTWWBTOHI-UHFFFAOYSA-N
Formula: C23H47NO
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 353.63

Physical Properties

Property code	Value	Unit	Source
gf	127.48	kJ/mol	Joback Method
hf	-571.85	kJ/mol	Joback Method
hfus	52.53	kJ/mol	Joback Method
hvap	74.29	kJ/mol	Joback Method
log10ws	-7.55		Crippen Method
logp	7.362		Crippen Method
mcvol	346.480	ml/mol	McGowan Method
pc	893.20	kPa	Joback Method
rinpol	2411.00		NIST Webbook
rinpol	2411.00		NIST Webbook
tb	788.72	K	Joback Method
tc	968.35	K	Joback Method
tf	433.79	K	Joback Method
vc	1.337	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1104.62	J/mol×K	788.72	Joback Method
cpg	1125.99	J/mol×K	818.66	Joback Method
cpg	1146.27	J/mol×K	848.60	Joback Method
cpg	1165.54	J/mol×K	878.53	Joback Method
cpg	1183.84	J/mol×K	908.47	Joback Method
cpg	1201.24	J/mol×K	938.41	Joback Method
cpg	1217.79	J/mol×K	968.35	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=U308131&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