Propanamide, N,N-dinonyl-2-methyl-

Inchi: InChI=1S/C22H45NO/c1-5-7-9-11-13-15-17-19-23(22(24)21(3)4)20-18-16-14-12-10-8-6-
InchiKey: KPJYYRFCGJJJLR-UHFFFAOYSA-N
Formula: C22H45NO
SMILES: CCCCCCCCCN(CCCCCCCCC)C(=O)C(C)C
Mol. weight [g/mol]: 339.60

Physical Properties

Property code	Value	Unit	Source
gf	113.78	kJ/mol	Joback Method
hf	-547.74	kJ/mol	Joback Method
hfus	53.83	kJ/mol	Joback Method
hvap	72.97	kJ/mol	Joback Method
log10ws	-7.14		Crippen Method
logp	6.972		Crippen Method
mcvol	332.390	ml/mol	McGowan Method
pc	940.37	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2355.00		NIST Webbook
tb	768.63	K	Joback Method
tc	944.19	K	Joback Method
tf	405.10	K	Joback Method
vc	1.286	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1041.63	J/mol×K	768.63	Joback Method
cpg	1062.65	J/mol×K	797.89	Joback Method
cpg	1082.65	J/mol×K	827.15	Joback Method
cpg	1101.65	J/mol×K	856.41	Joback Method
cpg	1119.70	J/mol×K	885.67	Joback Method
cpg	1136.84	J/mol×K	914.93	Joback Method
cpg	1153.12	J/mol×K	944.19	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308088&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