Propanamide, N,N-dioctyl-2,2-dimethyl-

Inchi: InChI=1S/C21H43NO/c1-6-8-10-12-14-16-18-22(20(23)21(3,4)5)19-17-15-13-11-9-7-2/h6
InchiKey: VLQKBOOLSUBTLT-UHFFFAOYSA-N
Formula: C21H43NO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C(C)(C)C
Mol. weight [g/mol]: 325.57

Physical Properties

Property code	Value	Unit	Source
gf	110.64	kJ/mol	Joback Method
hf	-530.57	kJ/mol	Joback Method
hfus	47.35	kJ/mol	Joback Method
hvap	69.83	kJ/mol	Joback Method
log10ws	-6.72		Crippen Method
logp	6.582		Crippen Method
mcvol	318.300	ml/mol	McGowan Method
pc	1005.26	kPa	Joback Method
rinpol	2205.00		NIST Webbook
rinpol	2205.00		NIST Webbook
tb	742.96	K	Joback Method
tc	917.86	K	Joback Method
tf	411.25	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.70	J/mol×K	742.96	Joback Method
cpg	1001.31	J/mol×K	772.11	Joback Method
cpg	1020.90	J/mol×K	801.26	Joback Method
cpg	1039.52	J/mol×K	830.41	Joback Method
cpg	1057.22	J/mol×K	859.56	Joback Method
cpg	1074.06	J/mol×K	888.71	Joback Method
cpg	1090.08	J/mol×K	917.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308130&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