Propanamide, N,N-dioctyl-2-methyl-

Inchi: InChI=1S/C20H41NO/c1-5-7-9-11-13-15-17-21(20(22)19(3)4)18-16-14-12-10-8-6-2/h19H
InchiKey: BJAXAJXLQZSAMF-UHFFFAOYSA-N
Formula: C20H41NO
SMILES: CCCCCCCCN(CCCCCCCC)C(=O)C(C)C
Mol. weight [g/mol]: 311.55

Physical Properties

Property code	Value	Unit	Source
gf	96.94	kJ/mol	Joback Method
hf	-506.46	kJ/mol	Joback Method
hfus	48.65	kJ/mol	Joback Method
hvap	68.52	kJ/mol	Joback Method
log10ws	-6.30		Crippen Method
logp	6.192		Crippen Method
mcvol	304.210	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	722.87	K	Joback Method
tc	893.90	K	Joback Method
tf	382.56	K	Joback Method
vc	1.173	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.91	J/mol×K	722.87	Joback Method
cpg	939.11	J/mol×K	751.37	Joback Method
cpg	958.36	J/mol×K	779.88	Joback Method
cpg	976.69	J/mol×K	808.38	Joback Method
cpg	994.14	J/mol×K	836.89	Joback Method
cpg	1010.74	J/mol×K	865.39	Joback Method
cpg	1026.52	J/mol×K	893.90	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=U308087&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