

Propanamide, 2-methyl-N-ethyl-N-tetradecyl-

Inchi:	InChI=1S/C20H41NO/c1-5-7-8-9-10-11-12-13-14-15-16-17-18-21(6-2)20(22)19(3)4/h19H
InchiKey:	CRRJUJWPCCCEJV-UHFFFAOYSA-N
Formula:	C20H41NO
SMILES:	CCCCCCCCCCCCCN(CC)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	2653.00		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/molxK	722.87	Joback Method
cpg	939.11	J/molxK	751.37	Joback Method
cpg	958.36	J/molxK	779.88	Joback Method
cpg	976.69	J/molxK	808.38	Joback Method
cpg	994.14	J/molxK	836.89	Joback Method
cpg	1010.74	J/molxK	865.39	Joback Method
cpg	1026.52	J/molxK	893.90	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415351&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

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
mccvol:	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

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