

Propanamide, 3-phenyl-N,N-diethyl-

Inchi:	InChI=1S/C13H19NO/c1-3-14(4-2)13(15)11-10-12-8-6-5-7-9-12/h5-9H,3-4,10-11H2,1-2H
InchiKey:	SEZMMTPBSLASLA-UHFFFAOYSA-N
Formula:	C13H19NO
SMILES:	CCN(CC)C(=O)CCc1ccccc1
Mol. weight [g/mol]:	205.30

Physical Properties

Property code	Value	Unit	Source
gf	152.85	kJ/mol	Joback Method
hf	-120.17	kJ/mol	Joback Method
hfus	28.09	kJ/mol	Joback Method
hvap	55.60	kJ/mol	Joback Method
log10ws	-2.71		Crippen Method
logp	2.488		Crippen Method
mcvol	181.820	ml/mol	McGowan Method
pc	2324.78	kPa	Joback Method
rinpol	1918.00		NIST Webbook
rinpol	1918.00		NIST Webbook
tb	589.83	K	Joback Method
tc	792.02	K	Joback Method
tf	345.09	K	Joback Method
vc	0.679	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	453.79	J/mol×K	589.83	Joback Method
cpg	470.40	J/mol×K	623.53	Joback Method
cpg	486.00	J/mol×K	657.23	Joback Method
cpg	500.66	J/mol×K	690.93	Joback Method
cpg	514.41	J/mol×K	724.62	Joback Method
cpg	527.30	J/mol×K	758.32	Joback Method
cpg	539.37	J/mol×K	792.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415389&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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