Propanamide, 3-phenyl-N-ethyl-N-methyl-

Inchi: InChI=1S/C12H17NO/c1-3-13(2)12(14)10-9-11-7-5-4-6-8-11/h4-8H,3,9-10H2,1-2H3
InchiKey: VZMRCYQQYXRRCJ-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: CCN(C)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 191.27

Physical Properties

Property code	Value	Unit	Source
gf	144.43	kJ/mol	Joback Method
hf	-99.53	kJ/mol	Joback Method
hfus	25.50	kJ/mol	Joback Method
hvap	53.37	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.098		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2555.92	kPa	Joback Method
rinpol	1879.00		NIST Webbook
rinpol	1879.00		NIST Webbook
tb	566.95	K	Joback Method
tc	772.19	K	Joback Method
tf	333.82	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.29	J/mol×K	566.95	Joback Method
cpg	420.36	J/mol×K	601.16	Joback Method
cpg	435.45	J/mol×K	635.36	Joback Method
cpg	449.60	J/mol×K	669.57	Joback Method
cpg	462.86	J/mol×K	703.78	Joback Method
cpg	475.27	J/mol×K	737.99	Joback Method
cpg	486.87	J/mol×K	772.19	Joback Method

Sources

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=U415388&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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