Propanamide, 3-phenyl-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C15H23NO/c1-4-16(12-13(2)3)15(17)11-10-14-8-6-5-7-9-14/h5-9,13H,4,10-12
InchiKey: LEOSSYMCQYJDIB-UHFFFAOYSA-N
Formula: C15H23NO
SMILES: CCN(CC(C)C)C(=O)CCc1ccccc1
Mol. weight [g/mol]: 233.35

Physical Properties

Property code	Value	Unit	Source
gf	167.25	kJ/mol	Joback Method
hf	-166.73	kJ/mol	Joback Method
hfus	29.74	kJ/mol	Joback Method
hvap	59.66	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	3.124		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1961.34	kPa	Joback Method
tb	635.15	K	Joback Method
tc	835.55	K	Joback Method
tf	352.63	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.61	J/mol×K	635.15	Joback Method
cpg	575.42	J/mol×K	668.55	Joback Method
cpg	592.16	J/mol×K	701.95	Joback Method
cpg	607.88	J/mol×K	735.35	Joback Method
cpg	622.63	J/mol×K	768.75	Joback Method
cpg	636.46	J/mol×K	802.15	Joback Method
cpg	649.43	J/mol×K	835.55	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415391&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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