Benzamide, 4-ethyl-N-butyl-N-methyl-

Inchi: InChI=1S/C14H21NO/c1-4-6-11-15(3)14(16)13-9-7-12(5-2)8-10-13/h7-10H,4-6,11H2,1-3
InchiKey: WKRWYUHJOLWAND-UHFFFAOYSA-N
Formula: C14H21NO
SMILES: CCCCN(C)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 219.32

Physical Properties

Property code	Value	Unit	Source
gf	151.64	kJ/mol	Joback Method
hf	-152.28	kJ/mol	Joback Method
hfus	30.29	kJ/mol	Joback Method
hvap	58.48	kJ/mol	Joback Method
log10ws	-3.67		Crippen Method
logp	3.121		Crippen Method
mcvol	195.910	ml/mol	McGowan Method
pc	2094.58	kPa	Joback Method
rinpol	2151.00		NIST Webbook
rinpol	2151.00		NIST Webbook
tb	617.69	K	Joback Method
tc	817.97	K	Joback Method
tf	368.88	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	504.68	J/mol×K	617.69	Joback Method
cpg	521.51	J/mol×K	651.07	Joback Method
cpg	537.37	J/mol×K	684.45	Joback Method
cpg	552.30	J/mol×K	717.83	Joback Method
cpg	566.34	J/mol×K	751.21	Joback Method
cpg	579.54	J/mol×K	784.59	Joback Method
cpg	591.92	J/mol×K	817.97	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=U415885&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