Benzamide, 4-ethyl-N-butyl-N-hexyl-

Inchi: InChI=1S/C19H31NO/c1-4-7-9-10-16-20(15-8-5-2)19(21)18-13-11-17(6-3)12-14-18/h11-1
InchiKey: NHKLKGVJUABGAR-UHFFFAOYSA-N
Formula: C19H31NO
SMILES: CCCCCCN(CCCC)C(=O)c1ccc(CC)cc1
Mol. weight [g/mol]: 289.46

Physical Properties

Property code	Value	Unit	Source
gf	193.74	kJ/mol	Joback Method
hf	-255.48	kJ/mol	Joback Method
hfus	43.24	kJ/mol	Joback Method
hvap	69.62	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.072		Crippen Method
mcvol	266.360	ml/mol	McGowan Method
pc	1408.01	kPa	Joback Method
rinpol	2752.00		NIST Webbook
rinpol	2752.00		NIST Webbook
tb	732.09	K	Joback Method
tc	923.01	K	Joback Method
tf	425.23	K	Joback Method
vc	1.016	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.17	J/mol×K	732.09	Joback Method
cpg	797.57	J/mol×K	763.91	Joback Method
cpg	814.94	J/mol×K	795.73	Joback Method
cpg	831.32	J/mol×K	827.55	Joback Method
cpg	846.77	J/mol×K	859.37	Joback Method
cpg	861.33	J/mol×K	891.19	Joback Method
cpg	875.05	J/mol×K	923.01	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=U415893&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