Benzamide, 4-butyl-N-hexyl-

Inchi: InChI=1S/C17H27NO/c1-3-5-7-8-14-18-17(19)16-12-10-15(11-13-16)9-6-4-2/h10-13H,3-
InchiKey: DSDPDFARXUYBOM-UHFFFAOYSA-N
Formula: C17H27NO
SMILES: CCCCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 261.40

Physical Properties

Property code	Value	Unit	Source
gf	155.51	kJ/mol	Joback Method
hf	-228.26	kJ/mol	Joback Method
hfus	40.14	kJ/mol	Joback Method
hvap	69.56	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.339		Crippen Method
mcvol	238.180	ml/mol	McGowan Method
pc	1655.15	kPa	Joback Method
rinpol	2305.00		NIST Webbook
rinpol	2305.00		NIST Webbook
tb	724.06	K	Joback Method
tc	920.66	K	Joback Method
tf	422.88	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.88	J/mol×K	724.06	Joback Method
cpg	701.95	J/mol×K	756.83	Joback Method
cpg	718.04	J/mol×K	789.59	Joback Method
cpg	733.19	J/mol×K	822.36	Joback Method
cpg	747.44	J/mol×K	855.12	Joback Method
cpg	760.83	J/mol×K	887.89	Joback Method
cpg	773.40	J/mol×K	920.66	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=U407452&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