

Benzamide, 4-butyl-N-octyl-

Inchi:	InChI=1S/C19H31NO/c1-3-5-7-8-9-10-16-20-19(21)18-14-12-17(13-15-18)11-6-4-2/h12-
InchiKey:	NEVRXRUEJPCMTR-UHFFFAOYSA-N
Formula:	C19H31NO
SMILES:	CCCCCCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	289.46

Physical Properties

Property code	Value	Unit	Source
gf	172.35	kJ/mol	Joback Method
hf	-269.54	kJ/mol	Joback Method
hfus	45.32	kJ/mol	Joback Method
hvap	74.01	kJ/mol	Joback Method
log10ws	-6.39		Crippen Method
logp	5.120		Crippen Method
mvol	266.360	ml/mol	McGowan Method
pc	1423.99	kPa	Joback Method
rinpol	2517.00		NIST Webbook
rinpol	2517.00		NIST Webbook
tb	769.82	K	Joback Method
tc	964.44	K	Joback Method
tf	445.42	K	Joback Method
vc	1.032	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	799.27	J/mol×K	769.82	Joback Method
cpg	816.88	J/mol×K	802.26	Joback Method
cpg	833.47	J/mol×K	834.69	Joback Method
cpg	849.09	J/mol×K	867.13	Joback Method
cpg	863.78	J/mol×K	899.57	Joback Method
cpg	877.60	J/mol×K	932.01	Joback Method
cpg	890.58	J/mol×K	964.44	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=U407455&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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