Benzamide, 4-butyl-N-nonyl-

Inchi: InChI=1S/C20H33NO/c1-3-5-7-8-9-10-11-17-21-20(22)19-15-13-18(14-16-19)12-6-4-2/h1
InchiKey: JZLBQLBIBSJCMO-UHFFFAOYSA-N
Formula: C20H33NO
SMILES: CCCCCCCCCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]: 303.48

Physical Properties

Property code	Value	Unit	Source
gf	180.77	kJ/mol	Joback Method
hf	-290.18	kJ/mol	Joback Method
hfus	47.91	kJ/mol	Joback Method
hvap	76.23	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	5.510		Crippen Method
mcvol	280.450	ml/mol	McGowan Method
pc	1326.17	kPa	Joback Method
rinpol	2622.00		NIST Webbook
rinpol	2622.00		NIST Webbook
tb	792.70	K	Joback Method
tc	987.17	K	Joback Method
tf	456.69	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.94	J/mol×K	792.70	Joback Method
cpg	875.79	J/mol×K	825.11	Joback Method
cpg	892.62	J/mol×K	857.52	Joback Method
cpg	908.45	J/mol×K	889.94	Joback Method
cpg	923.35	J/mol×K	922.35	Joback Method
cpg	937.35	J/mol×K	954.76	Joback Method
cpg	950.51	J/mol×K	987.17	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407456&Units=SI

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

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