

Benzamide, 2-methyl-N-butyl-N-octyl-

Inchi:	InChI=1S/C20H33NO/c1-4-6-8-9-10-13-17-21(16-7-5-2)20(22)19-15-12-11-14-18(19)3/h
InchiKey:	PSIJZQKNKVCQM-UHFFFAOYSA-N
Formula:	C20H33NO
SMILES:	CCCCCCCCN(CCCC)C(=O)c1ccccc1C
Mol. weight [g/mol]:	303.48

Physical Properties

Property code	Value	Unit	Source
gf	202.16	kJ/mol	Joback Method
hf	-276.12	kJ/mol	Joback Method
hfus	45.83	kJ/mol	Joback Method
hvap	71.84	kJ/mol	Joback Method
log10ws	-6.28		Crippen Method
logp	5.598		Crippen Method
mvol	280.450	ml/mol	McGowan Method
pc	1311.80	kPa	Joback Method
rinpol	3113.00		NIST Webbook
rinpol	3113.00		NIST Webbook
tb	754.97	K	Joback Method
tc	945.36	K	Joback Method
tf	436.50	K	Joback Method
vc	1.071	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.43	J/molxK	754.97	Joback Method
cpg	856.07	J/molxK	786.70	Joback Method
cpg	873.65	J/molxK	818.43	Joback Method
cpg	890.24	J/molxK	850.16	Joback Method
cpg	905.89	J/molxK	881.89	Joback Method
cpg	920.64	J/molxK	913.63	Joback Method
cpg	934.54	J/molxK	945.36	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=U415733&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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