

Benzamide, 4-methyl-N-butyl-N-propyl-

Inchi:	InChI=1S/C15H23NO/c1-4-6-12-16(11-5-2)15(17)14-9-7-13(3)8-10-14/h7-10H,4-6,11-12
InchiKey:	CHUDVKHJQQDKFM-UHFFFAOYSA-N
Formula:	C15H23NO
SMILES:	CCCCN(CCC)C(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	233.35

Physical Properties

Property code	Value	Unit	Source
gf	160.06	kJ/mol	Joback Method
hf	-172.92	kJ/mol	Joback Method
hfus	32.88	kJ/mol	Joback Method
hvap	60.71	kJ/mol	Joback Method
log10ws	-4.18		Crippen Method
logp	3.647		Crippen Method
mcvol	210.000	ml/mol	McGowan Method
pc	1921.98	kPa	Joback Method
rinsol	2914.00		NIST Webbook
tb	640.57	K	Joback Method
tc	838.24	K	Joback Method
tf	380.15	K	Joback Method
vc	0.791	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	557.07	J/mol×K	640.57	Joback Method
cpg	574.31	J/mol×K	673.52	Joback Method
cpg	590.57	J/mol×K	706.46	Joback Method
cpg	605.88	J/mol×K	739.41	Joback Method
cpg	620.29	J/mol×K	772.35	Joback Method
cpg	633.84	J/mol×K	805.30	Joback Method
cpg	646.58	J/mol×K	838.24	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=U415919&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
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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