Benzamide, 4-methyl-N-propyl-

Inchi: InChI=1S/C11H15NO/c1-3-8-12-11(13)10-6-4-9(2)5-7-10/h4-7H,3,8H2,1-2H3,(H,12,13)
InchiKey: MEKGGTFUDJLKHR-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]: 177.24

Physical Properties

Property code	Value	Unit	Source
gf	104.99	kJ/mol	Joback Method
hf	-104.42	kJ/mol	Joback Method
hfus	24.60	kJ/mol	Joback Method
hvap	56.20	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.135		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1684.00		NIST Webbook
tb	586.78	K	Joback Method
tc	799.33	K	Joback Method
tf	355.26	K	Joback Method
vc	0.585	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	370.75	J/mol×K	586.78	Joback Method
cpg	385.08	J/mol×K	622.20	Joback Method
cpg	398.56	J/mol×K	657.63	Joback Method
cpg	411.21	J/mol×K	693.05	Joback Method
cpg	423.07	J/mol×K	728.48	Joback Method
cpg	434.18	J/mol×K	763.90	Joback Method
cpg	444.55	J/mol×K	799.33	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=U407464&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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