N-Propyl-N-methyl-benzamide

Inchi: InChI=1S/C11H15NO/c1-3-9-12(2)11(13)10-7-5-4-6-8-10/h4-8H,3,9H2,1-2H3
InchiKey: AEYBXFRYLBPSBB-UHFFFAOYSA-N
Formula: C11H15NO
SMILES: CCCN(C)C(=O)c1ccccc1
Mol. weight [g/mol]: 177.24

Physical Properties

Property code	Value	Unit	Source
gf	136.01	kJ/mol	Joback Method
hf	-78.89	kJ/mol	Joback Method
hfus	22.91	kJ/mol	Joback Method
hvap	51.14	kJ/mol	Joback Method
log10ws	-2.45		Crippen Method
logp	2.169		Crippen Method
mcvol	153.640	ml/mol	McGowan Method
pc	2823.32	kPa	Joback Method
rinpol	1544.25		NIST Webbook
rinpol	1566.62		NIST Webbook
rinpol	1524.32		NIST Webbook
rinpol	1546.53		NIST Webbook
rinpol	1524.32		NIST Webbook
ripol	2476.34		NIST Webbook
ripol	2496.44		NIST Webbook
ripol	2456.51		NIST Webbook
tb	544.07	K	Joback Method
tc	752.53	K	Joback Method
tf	322.55	K	Joback Method
vc	0.568	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	356.38	J/mol×K	544.07	Joback Method
cpg	371.81	J/mol×K	578.81	Joback Method

cpg	386.29	J/mol×K	613.56	Joback Method
cpg	399.85	J/mol×K	648.30	Joback Method
cpg	412.53	J/mol×K	683.04	Joback Method
cpg	424.39	J/mol×K	717.79	Joback Method
cpg	435.45	J/mol×K	752.53	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=R194166&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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume