Benzamide, N-propyl-

Other names: N-(n-Propyl)benzamide
N-Propylbenzamide
Inchi: InChI=1S/C10H13NO/c1-2-8-11-10(12)9-6-4-3-5-7-9/h3-7H,2,8H2,1H3,(H,11,12)
InchiKey: DYZWXBMTHNHXML-UHFFFAOYSA-N
Formula: C10H13NO
SMILES: CCCNC(=O)c1ccccc1
Mol. weight [g/mol]: 163.22
CAS: 10546-70-0

Physical Properties

Property code	Value	Unit	Source
gf	106.20	kJ/mol	Joback Method
hf	-72.31	kJ/mol	Joback Method
hfus	22.39	kJ/mol	Joback Method
hvap	53.31	kJ/mol	Joback Method
log10ws	-2.65		Crippen Method
logp	1.826		Crippen Method
mcvol	139.550	ml/mol	McGowan Method
pc	3188.33	kPa	Joback Method
rinpol	1526.00		NIST Webbook
tb	558.92	K	Joback Method
tc	774.06	K	Joback Method
tf	331.47	K	Joback Method
vc	0.528	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	323.93	J/mol×K	558.92	Joback Method
cpg	337.81	J/mol×K	594.78	Joback Method
cpg	350.81	J/mol×K	630.63	Joback Method
cpg	362.97	J/mol×K	666.49	Joback Method
cpg	374.33	J/mol×K	702.34	Joback Method
cpg	384.93	J/mol×K	738.20	Joback Method

cpg	394.80	J/mol×K	774.06	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10546700&Units=SI
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

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