

N-benzyl-N-methyl-benzamide

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C15H15NO/c1-16(12-13-8-4-2-5-9-13)15(17)14-10-6-3-7-11-14/h2-11H,12H2,13H

UMDIHTNTVUNIDS-UHFFFAOYSA-N

C15H15NO

CN(Cc1ccccc1)C(=O)c1ccccc1

225.29

Physical Properties

Property code	Value	Unit	Source
gf	282.10	kJ/mol	Joback Method
hf	75.08	kJ/mol	Joback Method
hfus	27.31	kJ/mol	Joback Method
hvap	62.33	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.959		Crippen Method
mcvol	186.240	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
rinpol	1918.66		NIST Webbook
rinpol	1924.86		NIST Webbook
rinpol	1924.86		NIST Webbook
rinpol	1967.62		NIST Webbook
ripol	2634.98		NIST Webbook
ripol	2634.98		NIST Webbook
ripol	2732.45		NIST Webbook
ripol	2683.76		NIST Webbook
tb	662.27	K	Joback Method
tc	899.64	K	Joback Method
tf	394.05	K	Joback Method
vc	0.683	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	479.02	J/mol×K	662.27	Joback Method
cpg	495.53	J/mol×K	701.83	Joback Method

cpg	510.70	J/mol×K	741.39	Joback Method
cpg	524.62	J/mol×K	780.95	Joback Method
cpg	537.37	J/mol×K	820.52	Joback Method
cpg	549.06	J/mol×K	860.08	Joback Method
cpg	559.78	J/mol×K	899.64	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=R194057&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

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