N-(2-phenylethyl)-N-methyl-benzamide

Inchi: InChI=1S/C16H17NO/c1-17(13-12-14-8-4-2-5-9-14)16(18)15-10-6-3-7-11-15/h2-11H,12-
InchiKey: RIYFWDVINGTSQT-UHFFFAOYSA-N
Formula: C16H17NO
SMILES: CN(CCc1ccccc1)C(=O)c1ccccc1
Mol. weight [g/mol]: 239.31

Physical Properties

Property code	Value	Unit	Source
gf	290.52	kJ/mol	Joback Method
hf	54.44	kJ/mol	Joback Method
hfus	29.90	kJ/mol	Joback Method
hvap	64.55	kJ/mol	Joback Method
log10ws	-3.65		Crippen Method
logp	3.001		Crippen Method
mcvol	200.330	ml/mol	McGowan Method
pc	2424.27	kPa	Joback Method
rinpol	2072.18		NIST Webbook
rinpol	2029.09		NIST Webbook
rinpol	2077.79		NIST Webbook
rinpol	2029.09		NIST Webbook
rinpol	2023.03		NIST Webbook
ripol	2738.82		NIST Webbook
ripol	2836.64		NIST Webbook
ripol	2787.88		NIST Webbook
ripol	2738.82		NIST Webbook
tb	685.15	K	Joback Method
tc	917.78	K	Joback Method
tf	405.32	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.21	J/mol×K	685.15	Joback Method

cpg	548.03	J/mol×K	723.92	Joback Method
cpg	563.52	J/mol×K	762.69	Joback Method
cpg	577.78	J/mol×K	801.47	Joback Method
cpg	590.90	J/mol×K	840.24	Joback Method
cpg	602.95	J/mol×K	879.01	Joback Method
cpg	614.04	J/mol×K	917.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R194042&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

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