Benzamide, N-(4-methoxyphenyl)-3-methyl-

Inchi: InChI=1S/C15H15NO2/c1-11-4-3-5-12(10-11)15(17)16-13-6-8-14(18-2)9-7-13/h3-10H,1-
InchiKey: PFLGYHSIMYVEQR-UHFFFAOYSA-N
Formula: C15H15NO2
SMILES: COc1ccc(NC(=O)c2cccc(C)c2)cc1
Mol. weight [g/mol]: 241.29

Physical Properties

Property code	Value	Unit	Source
gf	136.45	kJ/mol	Joback Method
hf	-94.14	kJ/mol	Joback Method
hfus	29.80	kJ/mol	Joback Method
hvap	70.45	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.256		Crippen Method
mcvol	192.110	ml/mol	McGowan Method
pc	2584.59	kPa	Joback Method
rinpol	2328.00		NIST Webbook
rinpol	2328.00		NIST Webbook
tb	732.38	K	Joback Method
tc	969.14	K	Joback Method
tf	461.51	K	Joback Method
vc	0.719	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	516.70	J/mol×K	732.38	Joback Method
cpg	531.33	J/mol×K	771.84	Joback Method
cpg	544.80	J/mol×K	811.30	Joback Method
cpg	557.14	J/mol×K	850.76	Joback Method
cpg	568.42	J/mol×K	890.22	Joback Method
cpg	578.65	J/mol×K	929.68	Joback Method
cpg	587.90	J/mol×K	969.14	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=U307115&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

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