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

Inchi: InChI=1S/C15H15NO3/c1-18-13-8-6-12(7-9-13)16-15(17)11-4-3-5-14(10-11)19-2/h3-10H
InchiKey: RUAUMBFSLSSQDJ-UHFFFAOYSA-N
Formula: C15H15NO3
SMILES: COc1ccc(NC(=O)c2cccc(OC)c2)cc1
Mol. weight [g/mol]: 257.28

Physical Properties

Property code	Value	Unit	Source
gf	31.45	kJ/mol	Joback Method
hf	-226.36	kJ/mol	Joback Method
hfus	30.98	kJ/mol	Joback Method
hvap	72.86	kJ/mol	Joback Method
log10ws	-3.69		Crippen Method
logp	2.956		Crippen Method
mcvol	197.980	ml/mol	McGowan Method
pc	2540.49	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2467.00		NIST Webbook
tb	754.80	K	Joback Method
tc	988.32	K	Joback Method
tf	483.74	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	542.63	J/mol×K	754.80	Joback Method
cpg	556.80	J/mol×K	793.72	Joback Method
cpg	569.81	J/mol×K	832.64	Joback Method
cpg	581.67	J/mol×K	871.56	Joback Method
cpg	592.41	J/mol×K	910.48	Joback Method
cpg	602.05	J/mol×K	949.40	Joback Method
cpg	610.61	J/mol×K	988.32	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306970&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

https://www.chemeo.com/cid/93-517-5/Benzamide-N-4-methoxyphenyl-3-methoxy.pdf

Generated by Cheméo on 2024-10-12 09:09:09.580618679 +0000 UTC m=+3305012.217587927.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.