Benzamide, N-(4-methoxyphenyl)-4-ethyl-

Inchi: InChI=1S/C16H17NO2/c1-3-12-4-6-13(7-5-12)16(18)17-14-8-10-15(19-2)11-9-14/h4-11H
InchiKey: JGVYSRRKCKDZLQ-UHFFFAOYSA-N
Formula: C16H17NO2
SMILES: CCc1ccc(C(=O)Nc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 255.31

Physical Properties

Property code	Value	Unit	Source
gf	144.87	kJ/mol	Joback Method
hf	-114.78	kJ/mol	Joback Method
hfus	32.39	kJ/mol	Joback Method
hvap	72.68	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.510		Crippen Method
mcvol	206.200	ml/mol	McGowan Method
pc	2349.64	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	755.26	K	Joback Method
tc	987.67	K	Joback Method
tf	472.78	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	570.26	J/mol×K	755.26	Joback Method
cpg	585.21	J/mol×K	794.00	Joback Method
cpg	598.99	J/mol×K	832.73	Joback Method
cpg	611.63	J/mol×K	871.47	Joback Method
cpg	623.19	J/mol×K	910.20	Joback Method
cpg	633.71	J/mol×K	948.94	Joback Method
cpg	643.23	J/mol×K	987.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307016&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