N-(4-Methoxyphenethyl)benzamide

Inchi: InChI=1S/C16H17NO2/c1-19-15-9-7-13(8-10-15)11-12-17-16(18)14-5-3-2-4-6-14/h2-10H
InchiKey: RAOWOXJDGFFKKD-UHFFFAOYSA-N
Formula: C16H17NO2
SMILES: COc1ccc(CCNC(=O)c2ccccc2)cc1
Mol. weight [g/mol]: 255.31
CAS: 3278-19-1

Physical Properties

Property code	Value	Unit	Source
gf	154.50	kJ/mol	Joback Method
hf	-103.31	kJ/mol	Joback Method
hfus	32.77	kJ/mol	Joback Method
hvap	72.02	kJ/mol	Joback Method
log10ws	-3.97		Crippen Method
logp	2.668		Crippen Method
mcvol	206.200	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2363.20		NIST Webbook
rinpol	2363.20		NIST Webbook
tb	750.28	K	Joback Method
tc	981.93	K	Joback Method
tf	460.26	K	Joback Method
vc	0.774	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.36	J/mol×K	750.28	Joback Method
cpg	586.44	J/mol×K	788.89	Joback Method
cpg	600.32	J/mol×K	827.50	Joback Method
cpg	613.05	J/mol×K	866.10	Joback Method
cpg	624.70	J/mol×K	904.71	Joback Method
cpg	635.30	J/mol×K	943.32	Joback Method
cpg	644.92	J/mol×K	981.93	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3278191&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