Propanamide, N-(3-methoxyphenyl)-3-phenyl-

Inchi: InChI=1S/C16H17NO2/c1-19-15-10-8-14(9-11-15)17-16(18)12-7-13-5-3-2-4-6-13/h2-6,8-
InchiKey: JDXWZGXJTQCYCS-UHFFFAOYSA-N
Formula: C16H17NO2
SMILES: COc1ccc(NC(=O)CCc2ccccc2)cc1
Mol. weight [g/mol]: 255.31

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	-3.83		Crippen Method
logp	3.266		Crippen Method
mcvol	206.200	ml/mol	McGowan Method
pc	2384.19	kPa	Joback Method
rinpol	2366.00		NIST Webbook
rinpol	2366.00		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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308117&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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