Benzamide, N-(3-chlorophenyl)-3-methoxy-

Inchi: InChI=1S/C14H12ClNO2/c1-18-13-7-2-4-10(8-13)14(17)16-12-6-3-5-11(15)9-12/h2-9H,1
InchiKey: ZJTFEWWZCZJCIL-UHFFFAOYSA-N
Formula: C14H12ClNO2
SMILES: COc1cccc(C(=O)Nc2cccc(Cl)c2)c1
Mol. weight [g/mol]: 261.70

Physical Properties

Property code	Value	Unit	Source
gf	116.10	kJ/mol	Joback Method
hf	-89.24	kJ/mol	Joback Method
hfus	31.40	kJ/mol	Joback Method
hvap	72.61	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.601		Crippen Method
mcvol	190.260	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	2396.00		NIST Webbook
rinpol	2396.00		NIST Webbook
tb	746.93	K	Joback Method
tc	990.75	K	Joback Method
tf	480.16	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.90	J/mol×K	746.93	Joback Method
cpg	500.83	J/mol×K	787.57	Joback Method
cpg	512.63	J/mol×K	828.20	Joback Method
cpg	523.35	J/mol×K	868.84	Joback Method
cpg	533.05	J/mol×K	909.47	Joback Method
cpg	541.75	J/mol×K	950.11	Joback Method
cpg	549.51	J/mol×K	990.75	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U306969&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

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