Benzamide, N-(2,5-dimethoxyphenyl)-4-chloro-

Inchi: InChI=1S/C15H14ClNO3/c1-19-12-7-8-14(20-2)13(9-12)17-15(18)10-3-5-11(16)6-4-10/h
InchiKey: HCVYUDNPZQUVRH-UHFFFAOYSA-N
Formula: C15H14ClNO3
SMILES: COc1ccc(OC)c(NC(=O)c2ccc(Cl)cc2)c1
Mol. weight [g/mol]: 291.73

Physical Properties

Property code	Value	Unit	Source
gf	9.89	kJ/mol	Joback Method
hf	-253.57	kJ/mol	Joback Method
hfus	34.79	kJ/mol	Joback Method
hvap	77.91	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.610		Crippen Method
mcvol	210.220	ml/mol	McGowan Method
pc	2412.37	kPa	Joback Method
rinpol	2478.00		NIST Webbook
rinpol	2478.00		NIST Webbook
tb	797.21	K	Joback Method
tc	1033.87	K	Joback Method
tf	526.18	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	564.78	J/mol×K	797.21	Joback Method
cpg	577.52	J/mol×K	836.65	Joback Method
cpg	589.11	J/mol×K	876.10	Joback Method
cpg	599.56	J/mol×K	915.54	Joback Method
cpg	608.89	J/mol×K	954.98	Joback Method
cpg	617.12	J/mol×K	994.42	Joback Method
cpg	624.27	J/mol×K	1033.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307400&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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