2C-I

Other names: 4-iodo-2,5-dimethoxy-«beta»-phenethylamine
Inchi: InChI=1S/C10H14INO2/c1-13-9-6-8(11)10(14-2)5-7(9)3-4-12/h5-6H,3-4,12H2,1-2H3
InchiKey: PQHQBRJAAZQXHL-UHFFFAOYSA-N
Formula: C10H14INO2
SMILES: COc1cc(CCN)c(OC)cc1I
Mol. weight [g/mol]: 307.13
CAS: 64584-32-3

Physical Properties

Property code	Value	Unit	Source
gf	31.41	kJ/mol	Joback Method
hf	-201.39	kJ/mol	Joback Method
hfus	26.51	kJ/mol	Joback Method
hvap	66.95	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.810		Crippen Method
mcvol	175.540	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	2330.00		NIST Webbook
rinpol	2330.00		NIST Webbook
tb	680.33	K	Joback Method
tc	920.10	K	Joback Method
tf	452.22	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.26	J/mol×K	680.33	Joback Method
cpg	423.90	J/mol×K	720.29	Joback Method
cpg	435.74	J/mol×K	760.25	Joback Method
cpg	446.76	J/mol×K	800.21	Joback Method
cpg	456.97	J/mol×K	840.17	Joback Method
cpg	466.38	J/mol×K	880.14	Joback Method

cpg	474.97	J/mol×K	920.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64584323&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