2-(3',4'-Dimethoxyphenylethyl)-1,2,3,4-tetrahydroc

Inchi: InChI=1S/C19H23NO2/c1-21-18-12-8-14(13-19(18)22-2)7-10-16-11-9-15-5-3-4-6-17(15)
InchiKey: FYJFAAHVQJERQQ-UHFFFAOYSA-N
Formula: C19H23NO2
SMILES: COc1ccc(CCC2CCc3ccccc3N2)cc1OC
Mol. weight [g/mol]: 297.39

Physical Properties

Property code	Value	Unit	Source
gf	231.39	kJ/mol	Joback Method
hf	-156.83	kJ/mol	Joback Method
hfus	39.88	kJ/mol	Joback Method
hvap	76.09	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.063		Crippen Method
mcvol	241.910	ml/mol	McGowan Method
pc	1925.36	kPa	Joback Method
rinpol	2666.00		NIST Webbook
rinpol	2666.00		NIST Webbook
tb	806.82	K	Joback Method
tc	1043.47	K	Joback Method
tf	558.20	K	Joback Method
vc	0.905	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.36	J/mol×K	806.82	Joback Method
cpg	746.35	J/mol×K	846.26	Joback Method
cpg	762.89	J/mol×K	885.70	Joback Method
cpg	778.05	J/mol×K	925.14	Joback Method
cpg	791.85	J/mol×K	964.59	Joback Method
cpg	804.34	J/mol×K	1004.03	Joback Method
cpg	815.57	J/mol×K	1043.47	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R398224&Units=SI

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