2H-Pyran-2-one, 6-[2-(3,4-dimethoxyphenyl)ethyl]-5,6-dihydro-4-me (S)-

Other names: Tetrahydro-11-methoxyiangonin
(S)-6-(3,4-Dimethoxyphenethyl)-4-methoxy-5,6-dihydro-2H-pyran-2-one
Inchi: InChI=1S/C16H20O5/c1-18-13-9-12(21-16(17)10-13)6-4-11-5-7-14(19-2)15(8-11)20-3/h5
InchiKey: HEURTYMJWQPWNN-GFCCVEGCSA-N
Formula: C16H20O5
SMILES: COC1=CC(=O)OC(CCc2ccc(OC)c(OC)c2)C1
Mol. weight [g/mol]: 292.33
CAS: 38146-60-0

Physical Properties

Property code	Value	Unit	Source
gf	-301.94	kJ/mol	Joback Method
hf	-725.71	kJ/mol	Joback Method
hfus	34.18	kJ/mol	Joback Method
hvap	72.18	kJ/mol	Joback Method
log10ws	-3.33		Crippen Method
logp	2.482		Crippen Method
mcvol	222.430	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2615.30		NIST Webbook
rinpol	2615.30		NIST Webbook
tb	787.84	K	Joback Method
tc	1015.04	K	Joback Method
tf	503.68	K	Joback Method
vc	0.825	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	670.07	J/mol×K	787.84	Joback Method
cpg	686.92	J/mol×K	825.71	Joback Method
cpg	702.33	J/mol×K	863.57	Joback Method
cpg	716.23	J/mol×K	901.44	Joback Method
cpg	728.59	J/mol×K	939.31	Joback Method

cpg	739.36	J/mol×K	977.18	Joback Method
cpg	748.49	J/mol×K	1015.04	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C38146600&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

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