(E)-1-(3,4-dimethoxyphenyl)but-1-ene

Other names: (E)-1-(3',4'-Dimethoxyphenyl)but-1-ene
Inchi: InChI=1S/C12H16O2/c1-4-5-6-10-7-8-11(13-2)12(9-10)14-3/h5-9H,4H2,1-3H3/b6-5+
InchiKey: BONZIDALUXBFRW-AATRIKPKSA-N
Formula: C12H16O2
SMILES: CCC=Cc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 192.25

Physical Properties

Property code	Value	Unit	Source
gf	13.53	kJ/mol	Joback Method
hf	-224.64	kJ/mol	Joback Method
hfus	22.68	kJ/mol	Joback Method
hvap	50.68	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.127		Crippen Method
mcvol	163.620	ml/mol	McGowan Method
pc	2377.22	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1616.00		NIST Webbook
tb	559.60	K	Joback Method
tc	766.43	K	Joback Method
tf	315.84	K	Joback Method
vc	0.616	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	379.73	J/mol×K	559.60	Joback Method
cpg	394.80	J/mol×K	594.07	Joback Method
cpg	409.14	J/mol×K	628.54	Joback Method
cpg	422.75	J/mol×K	663.02	Joback Method
cpg	435.66	J/mol×K	697.49	Joback Method
cpg	447.87	J/mol×K	731.96	Joback Method
cpg	459.39	J/mol×K	766.43	Joback Method

dvisc	0.0010224	Pa×s	315.84	Joback Method
dvisc	0.0005757	Pa×s	356.47	Joback Method
dvisc	0.0003646	Pa×s	397.09	Joback Method
dvisc	0.0002513	Pa×s	437.72	Joback Method
dvisc	0.0001845	Pa×s	478.35	Joback Method
dvisc	0.0001422	Pa×s	518.97	Joback Method
dvisc	0.0001138	Pa×s	559.60	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=R504979&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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