trans-p-(1-Butenyl)-anisole

Inchi: InChI=1S/C11H14O/c1-3-4-5-10-6-8-11(12-2)9-7-10/h4-9H,3H2,1-2H3/b5-4+
InchiKey: XDQBFRZHMLRPGN-SNAWJCMRSA-N
Formula: C11H14O
SMILES: CCC=Cc1ccc(OC)cc1
Mol. weight [g/mol]: 162.23
CAS: 61866-52-2

Physical Properties

Property code	Value	Unit	Source
gf	119.74	kJ/mol	Joback Method
hf	-60.31	kJ/mol	Joback Method
hfus	19.29	kJ/mol	Joback Method
hvap	45.39	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.118		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2704.22	kPa	Joback Method
rinpol	1270.00		NIST Webbook
rinpol	1270.00		NIST Webbook
tb	509.32	K	Joback Method
tc	720.42	K	Joback Method
tf	269.82	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.52	J/mol×K	509.32	Joback Method
cpg	323.37	J/mol×K	544.50	Joback Method
cpg	337.42	J/mol×K	579.69	Joback Method
cpg	350.68	J/mol×K	614.87	Joback Method
cpg	363.20	J/mol×K	650.05	Joback Method
cpg	374.99	J/mol×K	685.23	Joback Method
cpg	386.09	J/mol×K	720.42	Joback Method

dvisc	0.0018064	Pa×s	269.82	Joback Method
dvisc	0.0009139	Pa×s	309.74	Joback Method
dvisc	0.0005401	Pa×s	349.65	Joback Method
dvisc	0.0003556	Pa×s	389.57	Joback Method
dvisc	0.0002530	Pa×s	429.49	Joback Method
dvisc	0.0001907	Pa×s	469.40	Joback Method
dvisc	0.0001503	Pa×s	509.32	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=C61866522&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