

2-Methoxy-4'-pentoxy-trans-stilbene

Inchi:	InChI=1S/C20H24O2/c1-3-4-7-16-22-19-14-11-17(12-15-19)10-13-18-8-5-6-9-20(18)21-2
InchiKey:	ZIQOVNYYJKVZOE-JLHYYAGUSA-N
Formula:	C20H24O2
SMILES:	CCCCCOc1ccc(C=Cc2ccccc2OC)cc1
Mol. weight [g/mol]:	296.40
CAS:	35135-43-4

Physical Properties

Property code	Value	Unit	Source
gf	193.30	kJ/mol	Joback Method
hf	-153.23	kJ/mol	Joback Method
hfus	37.44	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-5.99		Crippen Method
logp	5.435		Crippen Method
mcvol	252.580	ml/mol	McGowan Method
pc	1615.47	kPa	Joback Method
tb	769.32	K	Joback Method
tc	988.60	K	Joback Method
tf	435.00 ± 1.00	K	NIST Webbook
vc	0.956	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	722.03	J/mol×K	769.32	Joback Method
cpg	739.70	J/mol×K	805.87	Joback Method
cpg	756.16	J/mol×K	842.41	Joback Method
cpg	771.46	J/mol×K	878.96	Joback Method
cpg	785.64	J/mol×K	915.50	Joback Method
cpg	798.76	J/mol×K	952.05	Joback Method
cpg	810.86	J/mol×K	988.60	Joback Method
dvisc	0.0003035	Pa×s	488.57	Joback Method
dvisc	0.0005710	Pa×s	432.42	Joback Method

dvisc	0.0001837	Pa×s	544.72	Joback Method
dvisc	0.0001222	Pa×s	600.87	Joback Method
dvisc	0.0000871	Pa×s	657.02	Joback Method
dvisc	0.0000655	Pa×s	713.17	Joback Method
dvisc	0.0000514	Pa×s	769.32	Joback Method
hfust	41.17	kJ/mol	435.00	NIST Webbook
sfust	94.60	J/mol×K	435.00	NIST Webbook

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=C35135434&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
hfust:	Enthalpy of fusion at a given temperature
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
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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