

4-Methoxy-4'-heptoxy-trans-stilbene

Inchi:	InChI=1S/C22H28O2/c1-3-4-5-6-7-18-24-22-16-12-20(13-17-22)9-8-19-10-14-21(23-2)15
InchiKey:	NXFLCVCENJLQFQ-CMDGGGOBGSA-N
Formula:	C22H28O2
SMILES:	CCCCCCOC1CCC(C=Cc2ccc(OC)cc2)cc1
Mol. weight [g/mol]:	324.46
CAS:	35135-45-6

Physical Properties

Property code	Value	Unit	Source
gf	210.14	kJ/mol	Joback Method
hf	-194.51	kJ/mol	Joback Method
hfus	42.62	kJ/mol	Joback Method
hvap	75.22	kJ/mol	Joback Method
log10ws	-6.83		Crippen Method
logp	6.215		Crippen Method
mvol	280.760	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
tb	815.08	K	Joback Method
tc	1029.63	K	Joback Method
tf	423.00 ± 1.00	K	NIST Webbook
vc	1.067	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	837.62	J/mol×K	815.08	Joback Method
cpg	855.53	J/mol×K	850.84	Joback Method
cpg	872.22	J/mol×K	886.60	Joback Method
cpg	887.73	J/mol×K	922.36	Joback Method
cpg	902.12	J/mol×K	958.12	Joback Method
cpg	915.44	J/mol×K	993.88	Joback Method
cpg	927.74	J/mol×K	1029.63	Joback Method
dvisc	0.0002506	Paxs	514.98	Joback Method
dvisc	0.0004836	Paxs	454.96	Joback Method

dvisc	0.0001489	Paxs	575.00	Joback Method
dvisc	0.0000977	Paxs	635.02	Joback Method
dvisc	0.0000689	Paxs	695.04	Joback Method
dvisc	0.0000514	Paxs	755.06	Joback Method
dvisc	0.0000400	Paxs	815.08	Joback Method
hfust	42.76	kJ/mol	423.00	NIST Webbook
sfust	101.10	J/mol×K	423.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35135456&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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