4-Methoxy-4'-dodecoxy-trans-stilbene

Inchi: InChI=1S/C27H38O2/c1-3-4-5-6-7-8-9-10-11-12-23-29-27-21-17-25(18-22-27)14-13-24-1
InchiKey: ZTKXXACFPFBWBM-BUHFOSPRSA-N
Formula: C27H38O2
SMILES: CCCCCCCCCCCCOc1ccc(C=Cc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 394.59
CAS: 35135-49-0

Physical Properties

Property code	Value	Unit	Source
gf	252.24	kJ/mol	Joback Method
hf	-297.71	kJ/mol	Joback Method
hfus	55.57	kJ/mol	Joback Method
hvap	86.35	kJ/mol	Joback Method
log10ws	-8.92		Crippen Method
logp	8.165		Crippen Method
mcvol	351.210	ml/mol	McGowan Method
pc	1001.44	kPa	Joback Method
tb	929.48	K	Joback Method
tc	1143.72	K	Joback Method
tf	415.00 ± 1.00	K	NIST Webbook
vc	1.347	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1140.43	J/mol×K	929.48	Joback Method
cpg	1158.86	J/mol×K	965.19	Joback Method
cpg	1175.98	J/mol×K	1000.89	Joback Method
cpg	1191.86	J/mol×K	1036.60	Joback Method
cpg	1206.57	J/mol×K	1072.30	Joback Method
cpg	1220.17	J/mol×K	1108.01	Joback Method
cpg	1232.73	J/mol×K	1143.72	Joback Method
dvisc	0.0001438	Pa×s	581.00	Joback Method
dvisc	0.0002932	Pa×s	511.31	Joback Method

dvisc	0.0000821	Pa×s	650.70	Joback Method
dvisc	0.0000523	Pa×s	720.39	Joback Method
dvisc	0.0000360	Pa×s	790.09	Joback Method
dvisc	0.0000264	Pa×s	859.78	Joback Method
dvisc	0.0000203	Pa×s	929.48	Joback Method
hfust	58.66	kJ/mol	415.00	NIST Webbook
sfust	141.30	J/mol×K	415.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35135490&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
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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