4-Methoxy-4'-hexoxy-trans-stilbene

Inchi: InChI=1S/C21H26O2/c1-3-4-5-6-17-23-21-15-11-19(12-16-21)8-7-18-9-13-20(22-2)14-10
InchiKey: MWDBDMGQXOYWJG-BQYQJAHWSA-N
Formula: C21H26O2
SMILES: CCCCCCOc1ccc(C=Cc2ccc(OC)cc2)cc1
Mol. weight [g/mol]: 310.43
CAS: 35135-44-5

Physical Properties

Property code	Value	Unit	Source
gf	201.72	kJ/mol	Joback Method
hf	-173.87	kJ/mol	Joback Method
hfus	40.03	kJ/mol	Joback Method
hvap	72.99	kJ/mol	Joback Method
log10ws	-6.41		Crippen Method
logp	5.825		Crippen Method
mcvol	266.670	ml/mol	McGowan Method
pc	1497.67	kPa	Joback Method
tb	792.20	K	Joback Method
tc	1008.83	K	Joback Method
tf	430.00 ± 1.00	K	NIST Webbook
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	856.71	J/mol×K	972.73	Joback Method
cpg	843.47	J/mol×K	936.62	Joback Method
cpg	829.17	J/mol×K	900.52	Joback Method
cpg	813.76	J/mol×K	864.41	Joback Method
cpg	797.17	J/mol×K	828.31	Joback Method
cpg	779.37	J/mol×K	792.20	Joback Method
cpg	868.92	J/mol×K	1008.83	Joback Method
dvisc	0.0005270	Pa×s	443.69	Joback Method
dvisc	0.0000454	Pa×s	792.20	Joback Method

dvisc	0.0000581	Pa×s	734.12	Joback Method
dvisc	0.0000776	Pa×s	676.03	Joback Method
dvisc	0.0001095	Pa×s	617.94	Joback Method
dvisc	0.0001658	Pa×s	559.86	Joback Method
dvisc	0.0002765	Pa×s	501.78	Joback Method
hfust	41.38	kJ/mol	430.00	NIST Webbook
sfust	96.20	J/mol×K	430.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35135445&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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