«alpha»-Methyl-cis-stilbene

Inchi: InChI=1S/C15H14/c1-13(15-10-6-3-7-11-15)12-14-8-4-2-5-9-14/h2-12H,1H3/b13-12-
InchiKey: OVZXISBUYCEVEV-SEYXRHQNSA-N
Formula: C15H14
SMILES: CC(=Cc1ccccc1)c1ccccc1
Mol. weight [g/mol]: 194.27
CAS: 1017-22-7

Physical Properties

Property code	Value	Unit	Source
gf	371.91	kJ/mol	Joback Method
hf	227.56	kJ/mol	Joback Method
hfus	21.58	kJ/mol	Joback Method
hvap	53.57	kJ/mol	Joback Method
log10ws	-4.50		Crippen Method
logp	4.247		Crippen Method
mcvol	170.390	ml/mol	McGowan Method
pc	2659.77	kPa	Joback Method
tb	600.00	K	Joback Method
tc	850.12	K	Joback Method
tf	292.61	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.25	J/mol×K	600.00	Joback Method
cpg	419.27	J/mol×K	641.69	Joback Method
cpg	435.81	J/mol×K	683.37	Joback Method
cpg	450.99	J/mol×K	725.06	Joback Method
cpg	464.92	J/mol×K	766.75	Joback Method
cpg	477.72	J/mol×K	808.43	Joback Method
cpg	489.51	J/mol×K	850.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1017227&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume