«alpha»-tert.-Butoxystyrene

Inchi: InChI=1S/C12H16O/c1-10(13-12(2,3)4)11-8-6-5-7-9-11/h5-9H,1H2,2-4H3
InchiKey: FGYJVOVIGVLVBN-UHFFFAOYSA-N
Formula: C12H16O
SMILES: C=C(OC(C)(C)C)c1ccccc1
Mol. weight [g/mol]: 176.25

Physical Properties

Property code	Value	Unit	Source
gf	139.70	kJ/mol	Joback Method
hf	-79.81	kJ/mol	Joback Method
hfus	12.06	kJ/mol	Joback Method
hvap	45.11	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.472		Crippen Method
mcvol	157.750	ml/mol	McGowan Method
pc	2525.19	kPa	Joback Method
rinpol	1239.00		NIST Webbook
tb	516.39	K	Joback Method
tc	735.29	K	Joback Method
tf	260.35	K	Joback Method
vc	0.589	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.95	J/mol×K	516.39	Joback Method
cpg	373.30	J/mol×K	552.87	Joback Method
cpg	389.51	J/mol×K	589.36	Joback Method
cpg	404.65	J/mol×K	625.84	Joback Method
cpg	418.77	J/mol×K	662.33	Joback Method
cpg	431.93	J/mol×K	698.81	Joback Method
cpg	444.17	J/mol×K	735.29	Joback Method

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=R318080&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume