«alpha»-Isopropoxystyrene

Inchi: InChI=1S/C11H14O/c1-9(2)12-10(3)11-7-5-4-6-8-11/h4-9H,3H2,1-2H3
InchiKey: ZNZYLDJKNNOZEN-UHFFFAOYSA-N
Formula: C11H14O
SMILES: C=C(OC(C)C)c1ccccc1
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
gf	126.00	kJ/mol	Joback Method
hf	-55.70	kJ/mol	Joback Method
hfus	13.36	kJ/mol	Joback Method
hvap	43.79	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.082		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2755.56	kPa	Joback Method
rinpol	1193.00		NIST Webbook
tb	496.30	K	Joback Method
tc	709.72	K	Joback Method
tf	231.66	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.55	J/mol×K	496.30	Joback Method
cpg	323.24	J/mol×K	531.87	Joback Method
cpg	338.05	J/mol×K	567.44	Joback Method
cpg	352.01	J/mol×K	603.01	Joback Method
cpg	365.13	J/mol×K	638.58	Joback Method
cpg	377.47	J/mol×K	674.15	Joback Method
cpg	389.04	J/mol×K	709.72	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R318075&Units=SI

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