«beta»-Isopropoxystyrene, (E)

Inchi: InChI=1S/C11H14O/c1-10(2)12-9-8-11-6-4-3-5-7-11/h3-10H,1-2H3/b9-8+
InchiKey: VNOSMVIVSUHSPU-CMDGGOBGSA-N
Formula: C11H14O
SMILES: CC(C)OC=Cc1ccccc1
Mol. weight [g/mol]: 162.23

Physical Properties

Property code	Value	Unit	Source
gf	126.93	kJ/mol	Joback Method
hf	-54.12	kJ/mol	Joback Method
hfus	16.15	kJ/mol	Joback Method
hvap	44.34	kJ/mol	Joback Method
log10ws	-3.24		Crippen Method
logp	3.082		Crippen Method
mcvol	143.660	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
rinpol	1274.00		NIST Webbook
rinpol	1274.00		NIST Webbook
tb	503.90	K	Joback Method
tc	718.62	K	Joback Method
tf	242.30	K	Joback Method
vc	0.535	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.42	J/mol×K	503.90	Joback Method
cpg	324.08	J/mol×K	539.69	Joback Method
cpg	338.82	J/mol×K	575.47	Joback Method
cpg	352.68	J/mol×K	611.26	Joback Method
cpg	365.69	J/mol×K	647.05	Joback Method
cpg	377.90	J/mol×K	682.83	Joback Method
cpg	389.34	J/mol×K	718.62	Joback Method
dvisc	0.0037869	Pa×s	242.30	Joback Method

dvisc	0.0014587	Pa×s	285.90	Joback Method
dvisc	0.0007232	Pa×s	329.50	Joback Method
dvisc	0.0004225	Pa×s	373.10	Joback Method
dvisc	0.0002762	Pa×s	416.70	Joback Method
dvisc	0.0001957	Pa×s	460.30	Joback Method
dvisc	0.0001472	Pa×s	503.90	Joback Method

Sources

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=R318104&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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

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