(1-Propoxyethyl)benzene

Inchi: InChI=1S/C11H16O/c1-3-9-12-10(2)11-7-5-4-6-8-11/h4-8,10H,3,9H2,1-2H3
InchiKey: BHHQDDHLWBEJLT-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CCCOC(C)c1ccccc1
Mol. weight [g/mol]: 164.24
CAS: 91967-71-4

Physical Properties

Property code	Value	Unit	Source
gf	46.71	kJ/mol	Joback Method
hf	-171.34	kJ/mol	Joback Method
hfus	15.95	kJ/mol	Joback Method
hvap	56.70 ± 0.20	kJ/mol	NIST Webbook
log10ws	-3.08		Crippen Method
logp	3.174		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
tb	499.74	K	Joback Method
tc	704.63	K	Joback Method
tf	247.38	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.07	J/mol×K	704.63	Joback Method
cpg	325.73	J/mol×K	499.74	Joback Method
cpg	341.78	J/mol×K	533.89	Joback Method
cpg	357.01	J/mol×K	568.04	Joback Method
cpg	371.42	J/mol×K	602.19	Joback Method
cpg	385.06	J/mol×K	636.33	Joback Method
cpg	397.93	J/mol×K	670.48	Joback Method
dvisc	0.0001746	Pa×s	499.74	Joback Method
dvisc	0.0040450	Pa×s	247.38	Joback Method

dvisc	0.0016374	Pa×s	289.44	Joback Method
dvisc	0.0008338	Pa×s	331.50	Joback Method
dvisc	0.0004943	Pa×s	373.56	Joback Method
dvisc	0.0003257	Pa×s	415.62	Joback Method
dvisc	0.0002317	Pa×s	457.68	Joback Method
hvapt	56.40 ± 0.20	kJ/mol	304.50	NIST Webbook

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=C91967714&Units=SI

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
hvapt: Enthalpy of vaporization at a given temperature
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