O-sec-amylphenol

Other names: 2-(1-methylbutyl)phenol
Phenol, 2-(1-methylbutyl)-
Inchi: InChI=1S/C11H16O/c1-3-6-9(2)10-7-4-5-8-11(10)12/h4-5,7-9,12H,3,6H2,1-2H3
InchiKey: ROMXEVFSCNLHAB-UHFFFAOYSA-N
Formula: C11H16O
SMILES: CCCC(C)c1ccccc1O
Mol. weight [g/mol]: 164.24
CAS: 87-26-3

Physical Properties

Property code	Value	Unit	Source
gf	-2.91	kJ/mol	Joback Method
hf	-216.43	kJ/mol	Joback Method
hfus	20.55	kJ/mol	Joback Method
hvap	54.98	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.296		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
tb	515.74 ± 0.01	K	NIST Webbook
tc	777.32	K	Joback Method
tf	336.87	K	Joback Method
vc	0.503	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.84	J/mol×K	740.76	Joback Method
cpg	412.32	J/mol×K	704.20	Joback Method
cpg	400.05	J/mol×K	667.63	Joback Method
cpg	386.96	J/mol×K	631.07	Joback Method
cpg	372.96	J/mol×K	594.50	Joback Method
cpg	357.97	J/mol×K	557.94	Joback Method
cpg	434.70	J/mol×K	777.32	Joback Method

dvisc	0.0046044	Pa×s	336.87	Joback Method
dvisc	0.0000452	Pa×s	557.94	Joback Method
dvisc	0.0000744	Pa×s	521.10	Joback Method
dvisc	0.0001322	Pa×s	484.25	Joback Method
dvisc	0.0002578	Pa×s	447.41	Joback Method
dvisc	0.0005672	Pa×s	410.56	Joback Method
dvisc	0.0014575	Pa×s	373.72	Joback Method
hvapt	59.60	kJ/mol	449.00	NIST Webbook
hvapt	74.40	kJ/mol	449.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54521e+01
Coeff. B	-4.67166e+03
Coeff. C	-8.45260e+01
Temperature range (K), min.	392.59
Temperature range (K), max.	545.22

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C87263&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume