Benzene, propoxy-

Other names:	Ether, phenyl propyl
	Ether, propyl phenyl
	Phenyl propyl ether
	Propoxybenzene
	Propoxyphenyl
	Propyl phenyl ether
Inchi:	InChI=1S/C9H12O/c1-2-8-10-9-6-4-3-5-7-9/h3-7H,2,8H2,1H3
InchiKey:	DSNYFFJTZPIKFZ-UHFFFAOYSA-N
Formula:	C9H12O
SMILES:	CCCOc1ccccc1
Mol. weight [g/mol]:	136.19
CAS:	622-85-5

Physical Properties

Property code	Value	Unit	Source
gf	32.31	kJ/mol	Joback Method
hf	-124.78	kJ/mol	Joback Method
hfus	14.29	kJ/mol	Joback Method
hvap	40.31	kJ/mol	Joback Method
log10ws	-2.43		Crippen Method
logp	2.475		Crippen Method
mcvol	119.780	ml/mol	McGowan Method
pc	3199.16	kPa	Joback Method
rinpol	1078.00		NIST Webbook
rinpol	1089.00		NIST Webbook
rinpol	1064.70		NIST Webbook
rinpol	1064.70		NIST Webbook
ripol	1501.00		NIST Webbook
ripol	1506.00		NIST Webbook
tb	462.50 ± 0.50	K	NIST Webbook
tb	462.50 ± 0.50	K	NIST Webbook
tb	463.10	K	NIST Webbook
tb	463.05 ± 0.07	K	NIST Webbook
tc	660.22	K	Joback Method
tf	244.91 ± 0.05	K	NIST Webbook
tf	246.06 ± 0.30	K	NIST Webbook
tf	245.36 ± 0.50	K	NIST Webbook

vc	0.450	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	310.41	J/mol×K	660.22	Joback Method
cpg	300.02	J/mol×K	625.92	Joback Method
cpg	289.01	J/mol×K	591.62	Joback Method
cpg	277.38	J/mol×K	557.32	Joback Method
cpg	265.10	J/mol×K	523.02	Joback Method
cpg	252.16	J/mol×K	488.72	Joback Method
cpg	238.54	J/mol×K	454.42	Joback Method
dvisc	0.0027046	Pa×s	239.84	Joback Method
dvisc	0.0002037	Pa×s	454.42	Joback Method
dvisc	0.0002608	Pa×s	418.66	Joback Method
dvisc	0.0003496	Pa×s	382.89	Joback Method
dvisc	0.0004978	Pa×s	347.13	Joback Method
dvisc	0.0007687	Pa×s	311.37	Joback Method
dvisc	0.0013289	Pa×s	275.60	Joback Method
hvapt	46.50	kJ/mol	418.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.60100e+01
Coeff. B	-5.09038e+03
Coeff. C	-1.61990e+01
Temperature range (K), min.	339.96
Temperature range (K), max.	492.00

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=C622855&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

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