

Benzene, 1-ethyl-2-propyl-

Other names:	1-Ethyl-2-n-propylbenzene 1-Ethyl-2-propylbenzene o-propylethylbenzene
Inchi:	InChI=1S/C11H16/c1-3-7-11-9-6-5-8-10(11)4-2/h5-6,8-9H,3-4,7H2,1-2H3
InchiKey:	DMUVQFCRCMDZPW-UHFFFAOYSA-N
Formula:	C11H16
SMILES:	CCc1ccccc1CC
Mol. weight [g/mol]:	148.24
CAS:	16021-20-8

Physical Properties

Property code	Value	Unit	Source
gf	144.52	kJ/mol	Joback Method
hf	-45.31	kJ/mol	Joback Method
hfus	17.90	kJ/mol	Joback Method
hvap	43.02	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.202		Crippen Method
mcvol	142.090	ml/mol	McGowan Method
pc	2608.40	kPa	Joback Method
rinpol	1120.00		NIST Webbook
rinpol	1116.70		NIST Webbook
rinpol	1119.20		NIST Webbook
rinpol	1134.80		NIST Webbook
rinpol	1140.40		NIST Webbook
rinpol	1146.70		NIST Webbook
rinpol	1116.70		NIST Webbook
rinpol	1119.20		NIST Webbook
rinpol	1115.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1147.00		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1136.45		NIST Webbook
rinpol	1140.00		NIST Webbook

rinpol	1121.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1132.80		NIST Webbook
rinpol	1139.60		NIST Webbook
rinpol	1135.70		NIST Webbook
rinpol	1138.20		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1136.45		NIST Webbook
rinpol	1133.80		NIST Webbook
rinpol	1140.00		NIST Webbook
rinpol	1140.40		NIST Webbook
rinpol	1121.00		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1127.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1139.40		NIST Webbook
rinpol	1133.80		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1139.00		NIST Webbook
rinpol	1140.00		NIST Webbook
ripol	1363.50		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1363.50		NIST Webbook
ripol	1364.00		NIST Webbook
ripol	1364.00		NIST Webbook
tb	474.10 ± 2.00	K	NIST Webbook
tc	685.93	K	Joback Method
tf	252.67	K	Joback Method
vc	0.543	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	300.77	J/mol×K	482.74	Joback Method
cpg	371.23	J/mol×K	652.06	Joback Method
cpg	358.64	J/mol×K	618.20	Joback Method
cpg	345.33	J/mol×K	584.33	Joback Method
cpg	331.27	J/mol×K	550.47	Joback Method

cpg	316.42	J/mol×K	516.60	Joback Method
cpg	383.12	J/mol×K	685.93	Joback Method
dvisc	0.0002096	Paxs	482.74	Joback Method
dvisc	0.0002657	Paxs	444.39	Joback Method
dvisc	0.0003524	Paxs	406.05	Joback Method
dvisc	0.0004957	Paxs	367.71	Joback Method
dvisc	0.0007549	Paxs	329.36	Joback Method
dvisc	0.0012843	Paxs	291.01	Joback Method
dvisc	0.0025675	Paxs	252.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.44050e+01
Coeff. B	-3.94822e+03
Coeff. C	-7.27200e+01
Temperature range (K), min.	352.39
Temperature range (K), max.	506.90

Sources

The Yaws Handbook of Vapor Pressure:
Crippen Method:

<https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure>
<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C16021208&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
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

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