

Benzene, 1-ethyl-2-(phenylmethyl)-

Other names:	1-Ethyl-2-benzylbenzene 2'-Ethyldiphenylmethane 2-Ethyldiphenylmethane Methane, (o-ethylphenyl)phenyl-
Inchi:	InChI=1S/C15H16/c1-2-14-10-6-7-11-15(14)12-13-8-4-3-5-9-13/h3-11H,2,12H2,1H3
InchiKey:	SADTWSHFQKKIAT-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	CCc1cccc1Cc1cccc1
Mol. weight [g/mol]:	196.29
CAS:	28122-25-0

Physical Properties

Property code	Value	Unit	Source
chl	-8217.00	kJ/mol	NIST Webbook
gf	290.61	kJ/mol	Joback Method
hf	108.66	kJ/mol	Joback Method
hfus	22.30	kJ/mol	Joback Method
hvap	54.20	kJ/mol	Joback Method
log10ws	-4.37		Crippen Method
logp	3.840		Crippen Method
mcvol	174.690	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	274.00		NIST Webbook
rinpol	274.00		NIST Webbook
tb	564.01 ± 0.30	K	NIST Webbook
tc	836.65	K	Joback Method
tf	262.00 ± 0.20	K	NIST Webbook
vc	0.659	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.35	J/mol×K	600.94	Joback Method
cpg	499.09	J/mol×K	797.36	Joback Method

cpg	485.83	J/molxK	758.08	Joback Method
cpg	471.49	J/molxK	718.79	Joback Method
cpg	456.02	J/molxK	679.51	Joback Method
cpg	439.33	J/molxK	640.22	Joback Method
cpg	511.34	J/molxK	836.65	Joback Method
dvisc	0.0001619	Paxs	600.94	Joback Method
dvisc	0.0002059	Paxs	554.81	Joback Method
dvisc	0.0002736	Paxs	508.68	Joback Method
dvisc	0.0003847	Paxs	462.55	Joback Method
dvisc	0.0005833	Paxs	416.43	Joback Method
dvisc	0.0009812	Paxs	370.30	Joback Method
dvisc	0.0019137	Paxs	324.17	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46669e+01
Coeff. B	-4.76904e+03
Coeff. C	-8.94130e+01
Temperature range (K), min.	421.07
Temperature range (K), max.	599.17

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C28122250&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

chl: Standard liquid enthalpy of combustion

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

Latest version available from:

<https://www.cheméo.com/cid/39-440-0/Benzene-1-ethyl-2-phenylmethyl.pdf>

Generated by Cheméo on 2024-04-24 11:00:50.485659253 +0000 UTC m=+16245699.406236575.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.