

Benzene, 1-ethyl-3-(phenylmethyl)-

Other names:	1-Benzyl-3-ethylbenzene 3-Ethyldiphenylmethane
Inchi:	InChI=1S/C15H16/c1-2-13-9-6-10-15(11-13)12-14-7-4-3-5-8-14/h3-11H,2,12H2,1H3
InchiKey:	DITPGLQNHCMPAK-UHFFFAOYSA-N
Formula:	C15H16
SMILES:	CCc1cccc(Cc2ccccc2)c1
Mol. weight [g/mol]:	196.29
CAS:	28122-24-9

Physical Properties

Property code	Value	Unit	Source
chl	-8196.00	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	274.70		NIST Webbook
tb	564.69 ± 0.30	K	NIST Webbook
tc	836.65	K	Joback Method
tf	263.93 ± 0.20	K	NIST Webbook
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	421.35	J/mol×K	600.94	Joback Method
cpg	439.33	J/mol×K	640.22	Joback Method
cpg	456.02	J/mol×K	679.51	Joback Method
cpg	471.49	J/mol×K	718.79	Joback Method
cpg	485.83	J/mol×K	758.08	Joback Method

cpg	499.09	J/mol×K	797.36	Joback Method
cpg	511.34	J/mol×K	836.65	Joback Method
dvisc	0.0019137	Pa×s	324.17	Joback Method
dvisc	0.0009812	Pa×s	370.30	Joback Method
dvisc	0.0005833	Pa×s	416.43	Joback Method
dvisc	0.0003847	Pa×s	462.55	Joback Method
dvisc	0.0002736	Pa×s	508.68	Joback Method
dvisc	0.0002059	Pa×s	554.81	Joback Method
dvisc	0.0001619	Pa×s	600.94	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	1.46666e+01
Coeff. B	-4.77442e+03
Coeff. C	-8.95420e+01
Temperature range (K), min.	421.58
Temperature range (K), max.	599.89

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/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=C28122249&Units=SI>

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

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