

Undecane, 3-phenethyl-1-phenyl-

Other names:	1-Phenyl-3-(2'-phenylethyl)undecane 1-Phenyl-3-(2-phenethyl)hendecane 1-Phenyl-3-(2-phenethyl)undecane 1-Phenyl-3-(2-phenylethyl)hendecane 1-Phenyl-3-phenethylundecane Benzene, 1,1'-(3-octyl-1,5-pentanediy)bis-
Inchi:	InChI=1S/C25H36/c1-2-3-4-5-6-9-18-25(21-19-23-14-10-7-11-15-23)22-20-24-16-12-8-13
InchiKey:	KWXGNTNJHNGHDF-UHFFFAOYSA-N
Formula:	C25H36
SMILES:	CCCCCCCCC(CCc1ccccc1)CCc1ccccc1
Mol. weight [g/mol]:	336.55
CAS:	7225-70-9

Physical Properties

Property code	Value	Unit	Source
gf	382.00	kJ/mol	Joback Method
hf	-91.55	kJ/mol	Joback Method
hfus	45.06	kJ/mol	Joback Method
hvap	75.41	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	7.619		Crippen Method
mcvol	315.590	ml/mol	McGowan Method
pc	1150.65	kPa	Joback Method
tb	824.32	K	Joback Method
tc	1031.71	K	Joback Method
tf	409.35	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1085.96	J/mol×K	1031.71	Joback Method
cpg	982.49	J/mol×K	824.32	Joback Method
cpg	1002.65	J/mol×K	858.89	Joback Method

cpg	1021.53	J/mol×K	893.45	Joback Method
cpg	1039.22	J/mol×K	928.02	Joback Method
cpg	1055.80	J/mol×K	962.58	Joback Method
cpg	1071.35	J/mol×K	997.15	Joback Method
dvisc	0.0000482	Pa×s	824.32	Joback Method
dvisc	0.0014509	Pa×s	409.35	Joback Method
dvisc	0.0005458	Pa×s	478.51	Joback Method
dvisc	0.0002628	Pa×s	547.67	Joback Method
dvisc	0.0001491	Pa×s	616.84	Joback Method
dvisc	0.0000948	Pa×s	686.00	Joback Method
dvisc	0.0000655	Pa×s	755.16	Joback Method
hvapt	91.90	kJ/mol	488.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	$\ln(P_{vp}) = A + B/(T + C)$
Coeff. A	2.07562e+01
Coeff. B	-1.22496e+04
Coeff. C	7.79110e+01
Temperature range (K), min.	520.55
Temperature range (K), max.	715.22

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7225709&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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