Benzene, nonyl-

Other names:	1-PHENYLNONANE NONYLBENZENE Nonane, 1-phenyl- n-Nonylbenzene
Inchi:	InChI=1S/C15H24/c1-2-3-4-5-6-7-9-12-15-13-10-8-11-14-15/h8,10-11,13-14H,2-7,9,12H2
InchiKey:	LIXVMPBOGDCSRM-UHFFFAOYSA-N
Formula:	C15H24
SMILES:	CCCCCCCCCc1ccccc1
Mol. weight [g/mol]:	204.35
CAS:	1081-77-2

Physical Properties

Property code	Value	Unit	Source
af	0.6280		KDB
gf	187.83	kJ/mol	Joback Method
hf	-116.40	kJ/mol	Joback Method
hfus	28.65	kJ/mol	Joback Method
hvap	74.10 ± 0.50	kJ/mol	NIST Webbook
hvap	74.80	kJ/mol	NIST Webbook
log10ws	-5.20		Crippen Method
logp	4.980		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
nfpaf	%!d(float64=1)		KDB
pc	1900.00	kPa	KDB
rinpol	1542.80		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1552.20		NIST Webbook
rinpol	1556.98		NIST Webbook
rinpol	1560.39		NIST Webbook
rinpol	1570.95		NIST Webbook
rinpol	1576.27		NIST Webbook
rinpol	1579.75		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1554.10		NIST Webbook
rinpol	1559.50		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1542.80		NIST Webbook

rinpol	1555.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	265.60		NIST Webbook
rinpol	265.51		NIST Webbook
rinpol	265.60		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1554.10		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1554.00		NIST Webbook
ripol	1854.00		NIST Webbook
ripol	1847.00		NIST Webbook
ripol	1821.00		NIST Webbook
ripol	1854.00		NIST Webbook
tb	555.20	K	KDB
tc	741.00	K	KDB
tf	249.00	K	KDB
vc	0.790	m3/kmol	KDB
zc	0.2436270		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	492.55	J/mol×K	569.28	Joback Method
cpg	511.21	J/mol×K	601.21	Joback Method
cpg	528.89	J/mol×K	633.14	Joback Method
cpg	545.65	J/mol×K	665.07	Joback Method
cpg	561.51	J/mol×K	696.99	Joback Method
cpg	576.51	J/mol×K	728.92	Joback Method
cpg	590.69	J/mol×K	760.85	Joback Method
dvisc	0.0014881	Pa×s	332.57	Joback Method
dvisc	0.0035750	Pa×s	285.23	Joback Method
dvisc	0.0007706	Pa×s	379.91	Joback Method
dvisc	0.0004617	Pa×s	427.25	Joback Method
dvisc	0.0003064	Pa×s	474.60	Joback Method
dvisc	0.0002190	Pa×s	521.94	Joback Method
dvisc	0.0001656	Pa×s	569.28	Joback Method
hvapt	48.95	kJ/mol	555.20	KDB
hvapt	69.70	kJ/mol	365.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54330e+01
Coeff. B	-5.20756e+03
Coeff. C	-7.04730e+01
Temperature range (K), min.	414.31
Temperature range (K), max.	584.98

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.14515e+02
Coeff. B	-1.27354e+04
Coeff. C	-1.39957e+01
Coeff. D	4.83248e-06
Temperature range (K), min.	249.00
Temperature range (K), max.	741.00

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1081772&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=711
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
KDB:	https://www.cheric.org/files/research/kdb/mol/mol711.mol

Legend

af:	Acentric Factor
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
nfpaf:	NFPA Fire Rating
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
zc:	Critical Compressibility

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