

Benzene, (1-propylheptyl)-

Other names:	Decane, 4-phenyl- (4-Decyl)benzene (1-Propylheptyl)benzene
Inchi:	InChI=1S/C16H26/c1-3-5-6-8-12-15(11-4-2)16-13-9-7-10-14-16/h7,9-10,13-15H,3-6,8,11
InchiKey:	QTDBKYLPIZUTFN-UHFFFAOYSA-N
Formula:	C16H26
SMILES:	CCCCCCCC(CCC)c1ccccc1
Mol. weight [g/mol]:	218.38
CAS:	4537-12-6

Physical Properties

Property code	Value	Unit	Source
gf	193.81	kJ/mol	Joback Method
hf	-142.32	kJ/mol	Joback Method
hfus	27.71	kJ/mol	Joback Method
hvap	53.10	kJ/mol	Joback Method
log10ws	-5.59		Crippen Method
logp	5.541		Crippen Method
mcvol	212.540	ml/mol	McGowan Method
pc	1714.61	kPa	Joback Method
rinpol	264.40		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	264.40		NIST Webbook
rinpol	1538.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1743.00		NIST Webbook
ripol	1743.00		NIST Webbook
tb	591.72	K	Joback Method
tc	784.61	K	Joback Method
tf	281.50	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	545.09	J/mol×K	591.72	Joback Method
cpg	564.58	J/mol×K	623.87	Joback Method
cpg	583.04	J/mol×K	656.02	Joback Method
cpg	600.51	J/mol×K	688.17	Joback Method
cpg	617.03	J/mol×K	720.31	Joback Method
cpg	632.64	J/mol×K	752.46	Joback Method
cpg	647.38	J/mol×K	784.61	Joback Method
dvisc	0.0047483	Pa×s	281.50	Joback Method
dvisc	0.0016769	Pa×s	333.20	Joback Method
dvisc	0.0007833	Pa×s	384.91	Joback Method
dvisc	0.0004381	Pa×s	436.61	Joback Method
dvisc	0.0002772	Pa×s	488.31	Joback Method
dvisc	0.0001914	Pa×s	540.02	Joback Method
dvisc	0.0001410	Pa×s	591.72	Joback Method

Sources

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=C4537126&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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