Benzene, (1-ethylhexyl)-

Other names: Octane, 3-phenyl-
3-Phenyloctane
Inchi: InChI=1S/C14H22/c1-3-5-7-10-13(4-2)14-11-8-6-9-12-14/h6,8-9,11-13H,3-5,7,10H2,1-2H
InchiKey: XEYWPMIXBVMRLE-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCCC(CC)c1ccccc1
Mol. weight [g/mol]: 190.32
CAS: 18335-15-4

Physical Properties

Property code	Value	Unit	Source
gf	176.97	kJ/mol	Joback Method
hf	-101.04	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	48.65	kJ/mol	Joback Method
log10ws	-4.75		Crippen Method
logp	4.761		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	2023.58	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1366.00		NIST Webbook
rinpol	1358.00		NIST Webbook
rinpol	1355.00		NIST Webbook
rinpol	1352.00		NIST Webbook
tb	545.96	K	Joback Method
tc	744.01	K	Joback Method
tf	258.96	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.13	J/mol×K	545.96	Joback Method
cpg	460.73	J/mol×K	578.97	Joback Method

cpg	478.33	J/mol×K	611.98	Joback Method
cpg	494.96	J/mol×K	644.99	Joback Method
cpg	510.68	J/mol×K	678.00	Joback Method
cpg	525.51	J/mol×K	711.00	Joback Method
cpg	539.50	J/mol×K	744.01	Joback Method
dvisc	0.0053384	Pa×s	258.96	Joback Method
dvisc	0.0019183	Pa×s	306.79	Joback Method
dvisc	0.0009085	Pa×s	354.63	Joback Method
dvisc	0.0005139	Pa×s	402.46	Joback Method
dvisc	0.0003281	Pa×s	450.29	Joback Method
dvisc	0.0002284	Pa×s	498.13	Joback Method
dvisc	0.0001693	Pa×s	545.96	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C18335154&Units=SI
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

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
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume