Benzene, 1-ethyl-4-pentyl

Inchi: InChI=1S/C13H20/c1-3-5-6-7-13-10-8-12(4-2)9-11-13/h8-11H,3-7H2,1-2H3
InchiKey: LJFDIDJBEFXJKW-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCCCCc1ccc(CC)cc1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	161.36	kJ/mol	Joback Method
hf	-86.59	kJ/mol	Joback Method
hfus	23.08	kJ/mol	Joback Method
hvap	47.47	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	3.982		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2163.33	kPa	Joback Method
rinpol	1322.00		NIST Webbook
rinpol	1322.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1555.00		NIST Webbook
ripol	1563.30		NIST Webbook
tb	528.50	K	Joback Method
tc	726.20	K	Joback Method
tf	275.21	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.45	J/mol×K	528.50	Joback Method
cpg	471.14	J/mol×K	693.25	Joback Method
cpg	457.24	J/mol×K	660.30	Joback Method
cpg	442.55	J/mol×K	627.35	Joback Method
cpg	427.04	J/mol×K	594.40	Joback Method

cpg	410.68	J/mol×K	561.45	Joback Method
cpg	484.29	J/mol×K	726.20	Joback Method
dvisc	0.0001884	Pa×s	528.50	Joback Method
dvisc	0.0002417	Pa×s	486.28	Joback Method
dvisc	0.0003251	Pa×s	444.07	Joback Method
dvisc	0.0004654	Pa×s	401.86	Joback Method
dvisc	0.0007248	Pa×s	359.64	Joback Method
dvisc	0.0012700	Pa×s	317.42	Joback Method
dvisc	0.0026431	Pa×s	275.21	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R12476&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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