Benzene, 1-ethylpentyl

Other names: (1-Ethylpentyl)benzene
Inchi: InChI=1S/C13H20/c1-3-5-9-12(4-2)13-10-7-6-8-11-13/h6-8,10-12H,3-5,9H2,1-2H3
InchiKey: QXZANYPVYZTYBN-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCCCC(CC)c1ccccc1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	168.55	kJ/mol	Joback Method
hf	-80.40	kJ/mol	Joback Method
hfus	19.94	kJ/mol	Joback Method
hvap	46.42	kJ/mol	Joback Method
log10ws	-4.33		Crippen Method
logp	4.370		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2210.37	kPa	Joback Method
rinpol	1266.00		NIST Webbook
rinpol	1266.00		NIST Webbook
rinpol	1285.00		NIST Webbook
tb	523.08	K	Joback Method
tc	723.93	K	Joback Method
tf	247.69	K	Joback Method
vc	0.649	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.03	J/mol×K	523.08	Joback Method
cpg	411.05	J/mol×K	556.55	Joback Method
cpg	428.08	J/mol×K	590.03	Joback Method
cpg	444.18	J/mol×K	623.50	Joback Method
cpg	459.38	J/mol×K	656.98	Joback Method
cpg	473.71	J/mol×K	690.45	Joback Method

cpg	487.22	J/mol×K	723.93	Joback Method
dvisc	0.0055617	Pa×s	247.69	Joback Method
dvisc	0.0020186	Pa×s	293.59	Joback Method
dvisc	0.0009636	Pa×s	339.49	Joback Method
dvisc	0.0005486	Pa×s	385.38	Joback Method
dvisc	0.0003521	Pa×s	431.28	Joback Method
dvisc	0.0002461	Pa×s	477.18	Joback Method
dvisc	0.0001832	Pa×s	523.08	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R34&Units=SI

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

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