Benzene, 1,4-dimethyl-2-hexyl

Inchi: InChI=1S/C14H22/c1-4-5-6-7-8-14-11-12(2)9-10-13(14)3/h9-11H,4-8H2,1-3H3
InchiKey: HTZHBKUKVWJLEI-UHFFFAOYSA-N
Formula: C14H22
SMILES: CCCCCCc1cc(C)ccc1C
Mol. weight [g/mol]: 190.32

Physical Properties

Property code	Value	Unit	Source
gf	160.15	kJ/mol	Joback Method
hf	-118.70	kJ/mol	Joback Method
hfus	25.28	kJ/mol	Joback Method
hvap	50.36	kJ/mol	Joback Method
log10ws	-4.90		Crippen Method
logp	4.426		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1956.14	kPa	Joback Method
ripol	1743.00		NIST Webbook
ripol	1724.00		NIST Webbook
ripol	1718.00		NIST Webbook
ripol	1706.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1704.00		NIST Webbook
tb	556.36	K	Joback Method
tc	752.44	K	Joback Method
tf	299.00	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	442.90	J/mol×K	556.36	Joback Method
cpg	522.43	J/mol×K	719.76	Joback Method
cpg	508.14	J/mol×K	687.08	Joback Method
cpg	493.07	J/mol×K	654.40	Joback Method

cpg	477.19	J/mol×K	621.72	Joback Method
cpg	460.48	J/mol×K	589.04	Joback Method
cpg	535.97	J/mol×K	752.44	Joback Method
dvisc	0.0001713	Pa×s	556.36	Joback Method
dvisc	0.0002165	Pa×s	513.47	Joback Method
dvisc	0.0002856	Pa×s	470.57	Joback Method
dvisc	0.0003982	Pa×s	427.68	Joback Method
dvisc	0.0005979	Pa×s	384.79	Joback Method
dvisc	0.0009941	Pa×s	341.89	Joback Method
dvisc	0.0019127	Pa×s	299.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R556039&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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