Benzene, 1,4-dimethyl-2-pentyl

Inchi: InChI=1S/C13H20/c1-4-5-6-7-13-10-11(2)8-9-12(13)3/h8-10H,4-7H2,1-3H3
InchiKey: ROQGPVNKDWWQAW-UHFFFAOYSA-N
Formula: C13H20
SMILES: CCCCCc1cc(C)ccc1C
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
gf	151.73	kJ/mol	Joback Method
hf	-98.06	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	48.13	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.036		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2133.46	kPa	Joback Method
ripol	1609.00		NIST Webbook
ripol	1648.00		NIST Webbook
ripol	1608.00		NIST Webbook
ripol	1594.00		NIST Webbook
ripol	1624.00		NIST Webbook
ripol	1632.00		NIST Webbook
tb	533.48	K	Joback Method
tc	732.26	K	Joback Method
tf	287.73	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	393.98	J/mol×K	533.48	Joback Method
cpg	410.89	J/mol×K	566.61	Joback Method
cpg	426.98	J/mol×K	599.74	Joback Method
cpg	442.26	J/mol×K	632.87	Joback Method

cpg	456.76	J/mol×K	666.00	Joback Method
cpg	470.52	J/mol×K	699.13	Joback Method
cpg	483.54	J/mol×K	732.26	Joback Method
dvisc	0.0019117	Pa×s	287.73	Joback Method
dvisc	0.0010134	Pa×s	328.69	Joback Method
dvisc	0.0006184	Pa×s	369.65	Joback Method
dvisc	0.0004164	Pa×s	410.61	Joback Method
dvisc	0.0003012	Pa×s	451.56	Joback Method
dvisc	0.0002300	Pa×s	492.52	Joback Method
dvisc	0.0001830	Pa×s	533.48	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=R550066&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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