

Benzene, 1,2,4-trimethyl-5-pentyl

Inchi:	InChI=1S/C14H22/c1-5-6-7-8-14-10-12(3)11(2)9-13(14)4/h9-10H,5-8H2,1-4H3
InchiKey:	CVCUTPRPQSHDGA-UHFFFAOYSA-N
Formula:	C14H22
SMILES:	CCCCC1cc(C)c(C)cc1C
Mol. weight [g/mol]:	190.32

Physical Properties

Property code	Value	Unit	Source
gf	150.52	kJ/mol	Joback Method
hf	-130.17	kJ/mol	Joback Method
hfus	24.89	kJ/mol	Joback Method
hvap	51.02	kJ/mol	Joback Method
log10ws	-4.96		Crippen Method
logp	4.345		Crippen Method
mcvol	184.360	ml/mol	McGowan Method
pc	1930.44	kPa	Joback Method
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
rinpol	1252.00		NIST Webbook
tb	561.34	K	Joback Method
tc	758.43	K	Joback Method
tf	311.52	K	Joback Method
vc	0.712	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.27	J/molxK	561.34	Joback Method
cpg	460.57	J/molxK	594.19	Joback Method
cpg	477.05	J/molxK	627.04	Joback Method
cpg	492.74	J/molxK	659.89	Joback Method
cpg	507.66	J/molxK	692.73	Joback Method
cpg	521.83	J/molxK	725.58	Joback Method
cpg	535.27	J/molxK	758.43	Joback Method

dvisc	0.0014453	Paxs	311.52	Joback Method
dvisc	0.0008167	Paxs	353.16	Joback Method
dvisc	0.0005205	Paxs	394.79	Joback Method
dvisc	0.0003615	Paxs	436.43	Joback Method
dvisc	0.0002676	Paxs	478.07	Joback Method
dvisc	0.0002078	Paxs	519.70	Joback Method
dvisc	0.0001675	Paxs	561.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R258389&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

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