

1,4-Dimethyl-2,5-diethylbenzene

Inchi:	InChI=1S/C12H18/c1-5-11-7-10(4)12(6-2)8-9(11)3/h7-8H,5-6H2,1-4H3
InchiKey:	PJFFTZKKTDDFSE-UHFFFAOYSA-N
Formula:	C12H18
SMILES:	CCc1cc(C)c(CC)cc1C
Mol. weight [g/mol]:	162.27

Physical Properties

Property code	Value	Unit	Source
gf	133.68	kJ/mol	Joback Method
hf	-88.89	kJ/mol	Joback Method
hfus	19.71	kJ/mol	Joback Method
hvap	46.57	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.428		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2302.53	kPa	Joback Method
ripol	1494.80		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1495.00		NIST Webbook
tb	515.58	K	Joback Method
tc	718.31	K	Joback Method
tf	288.98	K	Joback Method
vc	0.600	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.28	J/mol×K	515.58	Joback Method
cpg	363.09	J/mol×K	549.37	Joback Method
cpg	378.15	J/mol×K	583.16	Joback Method
cpg	392.49	J/mol×K	616.94	Joback Method
cpg	406.14	J/mol×K	650.73	Joback Method
cpg	419.10	J/mol×K	684.52	Joback Method

cpg	431.41	J/mol×K	718.31	Joback Method
dvisc	0.0013949	Pa×s	288.98	Joback Method
dvisc	0.0008227	Pa×s	326.75	Joback Method
dvisc	0.0005414	Pa×s	364.51	Joback Method
dvisc	0.0003853	Pa×s	402.28	Joback Method
dvisc	0.0002908	Pa×s	440.05	Joback Method
dvisc	0.0002294	Pa×s	477.81	Joback Method
dvisc	0.0001874	Pa×s	515.58	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=R305643&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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