1,3-Dimethyl-2,5-diethylbenzene

Inchi: InChI=1S/C12H18/c1-5-11-7-9(3)12(6-2)10(4)8-11/h7-8H,5-6H2,1-4H3
InchiKey: QHEYGWMEGHDREV-UHFFFAOYSA-N
Formula: C12H18
SMILES: CCc1cc(C)c(CC)c(C)c1
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	1513.00		NIST Webbook
ripol	1513.40		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1513.00		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

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=R305603&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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