1,2,3-Trimethyl-4-isopropylbenzene

Inchi: InChI=1S/C12H18/c1-8(2)12-7-6-9(3)10(4)11(12)5/h6-8H,1-5H3
InchiKey: QHOPYXBAXVDHDW-UHFFFAOYSA-N
Formula: C12H18
SMILES: Cc1ccc(C(C)C)c(C)c1C
Mol. weight [g/mol]: 162.27

Physical Properties

Property code	Value	Unit	Source
gf	131.24	kJ/mol	Joback Method
hf	-94.17	kJ/mol	Joback Method
hfus	16.19	kJ/mol	Joback Method
hvap	46.18	kJ/mol	Joback Method
log10ws	-4.08		Crippen Method
logp	3.735		Crippen Method
mcvol	156.180	ml/mol	McGowan Method
pc	2320.31	kPa	Joback Method
ripol	1536.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1536.00		NIST Webbook
ripol	1536.00		NIST Webbook
tb	515.14	K	Joback Method
tc	722.37	K	Joback Method
tf	273.98	K	Joback Method
vc	0.594	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	347.52	J/mol×K	515.14	Joback Method
cpg	363.75	J/mol×K	549.68	Joback Method
cpg	379.20	J/mol×K	584.22	Joback Method
cpg	393.88	J/mol×K	618.76	Joback Method
cpg	407.83	J/mol×K	653.30	Joback Method
cpg	421.05	J/mol×K	687.83	Joback Method

cpg	433.58	J/mol×K	722.37	Joback Method
dvisc	0.0017985	Pa×s	273.98	Joback Method
dvisc	0.0009540	Pa×s	314.17	Joback Method
dvisc	0.0005843	Pa×s	354.37	Joback Method
dvisc	0.0003955	Pa×s	394.56	Joback Method
dvisc	0.0002877	Pa×s	434.75	Joback Method
dvisc	0.0002209	Pa×s	474.95	Joback Method
dvisc	0.0001767	Pa×s	515.14	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R305549&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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