1-ISOPROPYL-3-TERT-BUTYLBENZENE

Inchi: InChI=1S/C13H20/c1-10(2)11-7-6-8-12(9-11)13(3,4)5/h6-10H,1-5H3
InchiKey: OWOLIQXOOMFSJE-UHFFFAOYSA-N
Formula: C13H20
SMILES: CC(C)c1cccc(C(C)(C)C)c1
Mol. weight [g/mol]: 176.30

Physical Properties

Property code	Value	Unit	Source
af	0.3805		Cheméo Relay (1.0)
gf	161.76	kJ/mol	Joback Method
hf	-101.68	kJ/mol	Cheméo Relay (1.0)
hfus	12.14	kJ/mol	Joback Method
hvap	58.34	kJ/mol	Cheméo Relay (1.0)
ie	8.32	eV	Cheméo Relay (1.0)
log10ws	-5.31		Cheméo Relay (1.0)
logp	4.107		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2218.71	kPa	Joback Method
ripol	1397.00		NIST Webbook
ripol	1404.00		NIST Webbook
ripol	1431.00		NIST Webbook
ripol	1414.00		NIST Webbook
ripol	1406.00		NIST Webbook
tb	482.70 ± 1.00	K	NIST Webbook
tc	698.74	K	Cheméo Relay (1.0)
tf	238.34	K	Cheméo Relay (1.0)
vc	0.632	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	396.59	J/mol×K	524.83	Joback Method
cpg	493.91	J/mol×K	739.67	Joback Method
cpg	480.24	J/mol×K	703.86	Joback Method

cpg	465.63	J/mol×K	668.05	Joback Method
cpg	450.02	J/mol×K	632.25	Joback Method
cpg	433.35	J/mol×K	596.44	Joback Method
cpg	415.56	J/mol×K	560.64	Joback Method
dvisc	0.0005231	Pa×s	393.73	Joback Method
dvisc	0.0001675	Pa×s	524.83	Joback Method
dvisc	0.0002285	Pa×s	481.13	Joback Method
dvisc	0.0003317	Pa×s	437.43	Joback Method
dvisc	0.0050928	Pa×s	262.63	Joback Method
dvisc	0.0009242	Pa×s	350.03	Joback Method
dvisc	0.0019209	Pa×s	306.33	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C20033129&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

af: Acentric Factor
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
ie: Ionization energy
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