Benzene, 1,2,4-tris(1-methylethyl)-

Other names: Benzene, 1,2,4-tris(1-methylethyl)-
Inchi: InChI=1S/C15H24/c1-10(2)13-7-8-14(11(3)4)15(9-13)12(5)6/h7-12H,1-6H3
InchiKey: RWGMANKDYBWNNP-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC(C)c1ccc(C(C)C)c(C(C)C)c1
Mol. weight [g/mol]: 204.36

Physical Properties

Property code	Value	Unit	Source
af	0.4777		Cheméo Relay (1.0)
hf	-155.69	kJ/mol	Cheméo Relay (1.0)
hfus	17.30	kJ/mol	Joback Method
hvap	70.08	kJ/mol	Cheméo Relay (1.0)
ie	8.13	eV	Cheméo Relay (1.0)
log10ws	-5.99		Cheméo Relay (1.0)
logp	5.057		Crippen Method
mcvol	198.450	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	1201.00		NIST Webbook
ripol	1520.00		NIST Webbook
ripol	1540.00		NIST Webbook
ripol	1532.00		NIST Webbook
ripol	1528.00		NIST Webbook
ripol	1524.00		NIST Webbook
tb	517.20	K	NIST Webbook
tb	512.00 ± 2.00	K	NIST Webbook
tc	725.70	K	Cheméo Relay (1.0)
tf	312.15	K	Cheméo Relay (1.0)
vc	0.744	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	494.44	J/mol×K	577.92	Joback Method

cpg	596.23	J/mol×K	783.37	Joback Method
cpg	581.61	J/mol×K	749.13	Joback Method
cpg	566.10	J/mol×K	714.89	Joback Method
cpg	549.66	J/mol×K	680.65	Joback Method
cpg	532.26	J/mol×K	646.40	Joback Method
cpg	513.86	J/mol×K	612.16	Joback Method
dvisc	0.0004043	Pa×s	421.60	Joback Method
dvisc	0.0001301	Pa×s	577.92	Joback Method
dvisc	0.0001761	Pa×s	525.81	Joback Method
dvisc	0.0002549	Pa×s	473.70	Joback Method
dvisc	0.0047804	Pa×s	265.27	Joback Method
dvisc	0.0007301	Pa×s	369.49	Joback Method
dvisc	0.0016012	Pa×s	317.38	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	386.70	K	1.90	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C948323&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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

af: Acentric Factor
cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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