2,4-Diisopropyl toluene

Other names: 1-Methyl-2,4-diisopropylbenzene
Inchi: InChI=1S/C13H20/c1-9(2)12-7-6-11(5)13(8-12)10(3)4/h6-10H,1-5H3
InchiKey: LDBOQVVHBQWYRE-UHFFFAOYSA-N
Formula: C13H20
SMILES: Cc1ccc(C(C)C)cc1C(C)C
Mol. weight [g/mol]: 176.30
CAS: 1460-98-6

Physical Properties

Property code	Value	Unit	Source
gf	146.85	kJ/mol	Joback Method
hf	-108.62	kJ/mol	Joback Method
hfus	15.64	kJ/mol	Joback Method
hvap	47.36	kJ/mol	Joback Method
log10ws	-4.32		Crippen Method
logp	4.242		Crippen Method
mcvol	170.270	ml/mol	McGowan Method
pc	2165.35	kPa	Joback Method
ripol	1364.10		NIST Webbook
tb	532.60	K	Joback Method
tc	740.08	K	Joback Method
tf	257.73	K	Joback Method
vc	0.643	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	394.49	J/mol×K	532.60	Joback Method
cpg	474.53	J/mol×K	705.50	Joback Method
cpg	460.25	J/mol×K	670.92	Joback Method
cpg	445.14	J/mol×K	636.34	Joback Method
cpg	429.16	J/mol×K	601.76	Joback Method
cpg	412.29	J/mol×K	567.18	Joback Method
cpg	488.00	J/mol×K	740.08	Joback Method

dvisc	0.0001621	Pa×s	532.60	Joback Method
dvisc	0.0002128	Pa×s	486.79	Joback Method
dvisc	0.0002957	Pa×s	440.98	Joback Method
dvisc	0.0004434	Pa×s	395.17	Joback Method
dvisc	0.0007394	Pa×s	349.35	Joback Method
dvisc	0.0014389	Pa×s	303.54	Joback Method
dvisc	0.0035478	Pa×s	257.73	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.47705e+01
Coeff. B	-4.24149e+03
Coeff. C	-7.93580e+01
Temperature range (K), min.	372.22
Temperature range (K), max.	527.77

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1460986&Units=SI

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

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

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
pvap:	Vapor pressure
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume