2-(4-Isopropylphenyl)-2-propanol

Other names: Benzenemethanol, «alpha»,«alpha»-dimethyl-4-(1-methylethyl)-
«alpha»,«alpha»-Dimethyl-p-isopropylbenzyl alcohol
p-Hydroxydiisopropylbenzene
p-Oxidiisopropylbenzene
2-(4-Isopropylphenyl)-2-propanol

Inchi: InChI=1S/C12H18O/c1-9(2)10-5-7-11(8-6-10)12(3,4)13/h5-9,13H,1-4H3

InchiKey: VBSMBCNJCBKQFP-UHFFFAOYSA-N

Formula: C12H18O

SMILES: CC(C)c1ccc(C(C)(C)O)cc1

Mol. weight [g/mol]: 178.28

Physical Properties

Property code	Value	Unit	Source
af	0.6411		Cheméo Relay (1.0)
chs	-6950.90 ± 2.80	kJ/mol	NIST Webbook
gf	16.52	kJ/mol	Joback Method
hf	-256.73	kJ/mol	Cheméo Relay (1.0)
hfs	-343.70 ± 2.80	kJ/mol	NIST Webbook
hfus	13.64	kJ/mol	Joback Method
hvap	78.95	kJ/mol	Cheméo Relay (1.0)
ie	8.63	eV	Cheméo Relay (1.0)
log10ws	-3.02		Cheméo Relay (1.0)
logp	3.037		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2670.78	kPa	Joback Method
tb	506.83	K	Cheméo Relay (1.0)
tc	737.80	K	Cheméo Relay (1.0)
tf	336.73	K	Cheméo Relay (1.0)
vc	0.607	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.14	J/mol×K	763.37	Joback Method

cpg	485.79	J/mol×K	797.22	Joback Method
cpg	424.92	J/mol×K	627.98	Joback Method
cpg	438.71	J/mol×K	661.83	Joback Method
cpg	451.64	J/mol×K	695.68	Joback Method
cpg	463.77	J/mol×K	729.52	Joback Method
cpg	410.21	J/mol×K	594.13	Joback Method
dvisc	0.0008936	Pa×s	406.16	Joback Method
dvisc	0.0026894	Pa×s	359.17	Joback Method
dvisc	0.0112775	Pa×s	312.18	Joback Method
dvisc	0.0003731	Pa×s	453.15	Joback Method
dvisc	0.0001836	Pa×s	500.15	Joback Method
dvisc	0.0001020	Pa×s	547.14	Joback Method
dvisc	0.0000622	Pa×s	594.13	Joback Method
hsubt	100.80 ± 1.80	kJ/mol	302.00	NIST Webbook

Sources

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):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3445429&Units=SI

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

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

Legend

af: Acentric Factor

chs: Standard solid enthalpy of combustion

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf: Standard Gibbs free energy of formation

hf: Enthalpy of formation at standard conditions

hfs: Solid phase enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hsubt: Enthalpy of sublimation at a given temperature

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume