Propofol

Other names:	Phenol, 2,6-bis(1-methylethyl)-
	Phenol, 2,6-diisopropyl-
	2,6-Diisopropylphenol
	Diprivan
	ICI 35868
	2,6-Bis(1-methylethyl)phenol
	Disoprofol
	Disoprivan
	Rapinovet
	2,6-bis(Isopropyl)phenol
	Ampofol
	Aquafol
	Diprifusor
	Diprivan 10
	Diprofol
	Fresofol
	Ivofol
	NSC 5105
	Pofol
	Propofol-lipuro
	Propovan
	Recofol
Inchi:	InChI=1S/C12H18O/c1-8(2)10-6-5-7-11(9(3)4)12(10)13/h5-9,13H,1-4H3
InchiKey:	OLBCVFGFOZPWHH-UHFFFAOYSA-N
Formula:	C12H18O
SMILES:	CC(C)c1cccc(C(C)C)c1O
Mol. weight [g/mol]:	178.27
CAS:	2078-54-8

Physical Properties

Property code	Value	Unit	Source
chl	-6962.00	kJ/mol	NIST Webbook
gf	-6.56	kJ/mol	Joback Method
hf	-244.40	kJ/mol	NIST Webbook
hf	-254.10 ± 2.80	kJ/mol	NIST Webbook
hfl	-330.00	kJ/mol	NIST Webbook

hfus	19.22	kJ/mol	Joback Method
hvap	68.70 ± 0.30	kJ/mol	NIST Webbook
hvap	86.11	kJ/mol	NIST Webbook
hvap	85.60	kJ/mol	NIST Webbook
log10ws	-3.39		Crippen Method
logp	3.639		Crippen Method
mcvol	162.050	ml/mol	McGowan Method
pc	2802.44	kPa	Joback Method
rinpol	1364.80		NIST Webbook
rinpol	1361.10		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1335.00		NIST Webbook
rinpol	235.30		NIST Webbook
rinpol	1346.00		NIST Webbook
rinpol	1364.80		NIST Webbook
rinpol	1362.70		NIST Webbook
rinpol	1334.60		NIST Webbook
rinpol	1365.60		NIST Webbook
ripol	1992.00		NIST Webbook
tb	585.36	K	Joback Method
tc	806.59	K	Joback Method
tf	345.66	K	Joback Method
vc	0.553	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	475.53	J/mol×K	769.72	Joback Method
cpg	450.20	J/mol×K	695.97	Joback Method
cpg	436.33	J/mol×K	659.10	Joback Method
cpg	421.56	J/mol×K	622.23	Joback Method
cpg	405.79	J/mol×K	585.36	Joback Method
cpg	463.24	J/mol×K	732.85	Joback Method
cpg	487.16	J/mol×K	806.59	Joback Method
dvisc	0.0036943	Pa×s	345.66	Joback Method
dvisc	0.0000319	Pa×s	585.36	Joback Method
dvisc	0.0000527	Pa×s	545.41	Joback Method
dvisc	0.0000943	Pa×s	505.46	Joback Method
dvisc	0.0001862	Pa×s	465.51	Joback Method
dvisc	0.0004182	Pa×s	425.56	Joback Method
dvisc	0.0011103	Pa×s	385.61	Joback Method

hfust	14.64	kJ/mol	292.80	NIST Webbook
hfust	14.64	kJ/mol	292.80	NIST Webbook
hvapt	67.90 ± 0.30	kJ/mol	310.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	529.20	K	102.00	NIST Webbook

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2078548&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl: Standard liquid 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
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hfust: Enthalpy of fusion at a given temperature
hvap: Enthalpy of vaporization at standard conditions
hvapt: Enthalpy of vaporization at a given temperature
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