

1,2-Dimethoxy-4-propylbenzene

Other names:	Benzene, 1,2-dimethoxy-4-propyl- Dihydromethyleugenol 1,2-Dimethoxy-4-propylbenzene
Inchi:	InChI=1S/C11H16O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h6-8H,4-5H2,1-3H3
InchiKey:	YXLFQKUIZVSIEP-UHFFFAOYSA-N
Formula:	C11H16O2
SMILES:	CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]:	180.25

Physical Properties

Property code	Value	Unit	Source
af	0.5770		Cheméo Relay (1.0)
hfus	19.89	kJ/mol	Joback Method
hvap	68.50	kJ/mol	Cheméo Relay (1.0)
ie	7.88	eV	Cheméo Relay (1.0)
log10ws	-3.12		Cheméo Relay (1.0)
logp	2.656		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	521.38	K	Cheméo Relay (1.0)
tc	711.41	K	Cheméo Relay (1.0)
tf	288.61	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.48	J/mol×K	532.56	Joback Method
cpg	430.10	J/mol×K	733.53	Joback Method
cpg	418.55	J/mol×K	700.03	Joback Method
cpg	406.38	J/mol×K	666.54	Joback Method
cpg	393.58	J/mol×K	633.04	Joback Method
cpg	380.17	J/mol×K	599.55	Joback Method
cpg	366.13	J/mol×K	566.05	Joback Method
dvisc	0.0003060	Pa×s	421.10	Joback Method

dvisc	0.0001437	Pa×s	532.56	Joback Method
dvisc	0.0001780	Pa×s	495.41	Joback Method
dvisc	0.0002283	Pa×s	458.26	Joback Method
dvisc	0.0011230	Pa×s	309.65	Joback Method
dvisc	0.0004340	Pa×s	383.95	Joback Method
dvisc	0.0006634	Pa×s	346.80	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5888528&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):

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point

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