

1,2-Dimethoxy-4-n-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]:	180.24
CAS:	5888-52-8

Physical Properties

Property code	Value	Unit	Source
gf	-75.11	kJ/mol	Joback Method
hf	-321.22	kJ/mol	Joback Method
hfus	19.89	kJ/mol	Joback Method
hvap	48.50	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.656		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2482.59	kPa	Joback Method
tb	532.56	K	Joback Method
tc	733.53	K	Joback Method
tf	309.65	K	Joback Method
vc	0.580	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

cpg	430.10	J/molxK	733.53	Joback Method
dvisc	0.0011230	Paxs	309.65	Joback Method
dvisc	0.0006634	Paxs	346.80	Joback Method
dvisc	0.0004340	Paxs	383.95	Joback Method
dvisc	0.0003060	Paxs	421.10	Joback Method
dvisc	0.0002283	Paxs	458.26	Joback Method
dvisc	0.0001780	Paxs	495.41	Joback Method
dvisc	0.0001437	Paxs	532.56	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.00 ± 1.00	K	2.70	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=C5888528&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
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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