Dihydromethyleugenol

Other names: 1,2-Dimethoxy-4-propylbenzene
Inchi: InChI=1S/C11H16O2/c1-4-5-9-6-7-10(12-2)11(8-9)13-3/h4,6-8,10-11H,1,5H2,2-3H3
InchiKey: LQSVMIMIFSSFGG-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: C=CCC1=CC(OC)C(OC)C=C1
Mol. weight [g/mol]: 180.24
CAS: 69780-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-13.39	kJ/mol	Joback Method
hf	-271.31	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	45.60	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.089		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1515.00		NIST Webbook
rinpol	1515.00		NIST Webbook
ripol	2725.00		NIST Webbook
ripol	2725.00		NIST Webbook
tb	510.78	K	Joback Method
tc	711.37	K	Joback Method
tf	273.61	K	Joback Method
vc	0.573	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.74	J/mol×K	510.78	Joback Method
cpg	368.28	J/mol×K	544.21	Joback Method
cpg	384.09	J/mol×K	577.64	Joback Method
cpg	399.19	J/mol×K	611.08	Joback Method

cpg	413.57	J/mol×K	644.51	Joback Method
cpg	427.22	J/mol×K	677.94	Joback Method
cpg	440.15	J/mol×K	711.37	Joback Method
dvisc	0.0012893	Pa×s	273.61	Joback Method
dvisc	0.0007553	Pa×s	313.14	Joback Method
dvisc	0.0004988	Pa×s	352.67	Joback Method
dvisc	0.0003582	Pa×s	392.19	Joback Method
dvisc	0.0002733	Pa×s	431.72	Joback Method
dvisc	0.0002182	Pa×s	471.25	Joback Method
dvisc	0.0001804	Pa×s	510.78	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C69780730&Units=SI

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

rinpol: Non-polar retention indices

ripol: Polar retention indices

tb: Normal Boiling Point Temperature

tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume