1,2,6-trimethoxy-4-propylbenzene

Inchi: InChI=1S/C12H18O3/c1-5-6-9-7-10(13-2)12(15-4)11(8-9)14-3/h7-8H,5-6H2,1-4H3
InchiKey: AOVUTAOJQZOAGA-UHFFFAOYSA-N
Formula: C12H18O3
SMILES: CCCc1cc(OC)c(OC)c(OC)c1
Mol. weight [g/mol]: 210.27

Physical Properties

Property code	Value	Unit	Source
gf	-181.32	kJ/mol	Joback Method
hf	-485.55	kJ/mol	Joback Method
hfus	23.27	kJ/mol	Joback Method
hvap	53.80	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.665		Crippen Method
mcvol	173.790	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1730.00		NIST Webbook
rinpol	1730.00		NIST Webbook
tb	582.84	K	Joback Method
tc	780.29	K	Joback Method
tf	355.67	K	Joback Method
vc	0.653	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	424.58	J/mol×K	582.84	Joback Method
cpg	439.63	J/mol×K	615.75	Joback Method
cpg	454.08	J/mol×K	648.66	Joback Method
cpg	467.91	J/mol×K	681.57	Joback Method
cpg	481.11	J/mol×K	714.47	Joback Method
cpg	493.65	J/mol×K	747.38	Joback Method
cpg	505.52	J/mol×K	780.29	Joback Method
dvisc	0.0006752	Pa×s	355.67	Joback Method

dvisc	0.0004279	Pa×s	393.53	Joback Method
dvisc	0.0002938	Pa×s	431.39	Joback Method
dvisc	0.0002143	Pa×s	469.25	Joback Method
dvisc	0.0001639	Pa×s	507.12	Joback Method
dvisc	0.0001301	Pa×s	544.98	Joback Method
dvisc	0.0001064	Pa×s	582.84	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R322222&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

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