2,5-Dimetoxycymene

Inchi: InChI=1S/C11H16O2/c1-8(2)10-7-9(12-3)5-6-11(10)13-4/h5-8H,1-4H3
InchiKey: UOMQSUCWUDELOW-UHFFFAOYSA-N
Formula: C11H16O2
SMILES: COc1ccc(OC)c(C(C)C)c1
Mol. weight [g/mol]: 180.24

Physical Properties

Property code	Value	Unit	Source
gf	-77.55	kJ/mol	Joback Method
hf	-326.50	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	48.11	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.827		Crippen Method
mcvol	153.830	ml/mol	McGowan Method
pc	2502.50	kPa	Joback Method
rinpol	1399.00		NIST Webbook
rinpol	1399.00		NIST Webbook
ripol	1852.00		NIST Webbook
ripol	1852.00		NIST Webbook
tb	532.12	K	Joback Method
tc	737.45	K	Joback Method
tf	294.65	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	351.77	J/mol×K	532.12	Joback Method
cpg	366.81	J/mol×K	566.34	Joback Method
cpg	381.19	J/mol×K	600.56	Joback Method
cpg	394.92	J/mol×K	634.78	Joback Method
cpg	407.99	J/mol×K	669.00	Joback Method
cpg	420.40	J/mol×K	703.22	Joback Method

cpg	432.15	J/mol×K	737.45	Joback Method
dvisc	0.0014340	Pa×s	294.65	Joback Method
dvisc	0.0007663	Pa×s	334.23	Joback Method
dvisc	0.0004676	Pa×s	373.81	Joback Method
dvisc	0.0003137	Pa×s	413.38	Joback Method
dvisc	0.0002256	Pa×s	452.96	Joback Method
dvisc	0.0001711	Pa×s	492.54	Joback Method
dvisc	0.0001352	Pa×s	532.12	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R518186&Units=SI

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