

Phenethyl alcohol, 2,5-dimethoxy-alpha-methyl-

Inchi:	InChI=1S/C11H16O3/c1-8(12)6-9-7-10(13-2)4-5-11(9)14-3/h4-5,7-8,12H,6H2,1-3H3
InchiKey:	RPYWIZDAMGNPJB-UHFFFAOYSA-N
Formula:	C11H16O3
SMILES:	COc1ccc(OC)c(CC(C)O)c1
Mol. weight [g/mol]:	196.24
CAS:	40180-96-9

Physical Properties

Property code	Value	Unit	Source
gf	-214.37	kJ/mol	Joback Method
hf	-478.73	kJ/mol	Joback Method
hfus	20.45	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	1.627		Crippen Method
mcvol	159.700	ml/mol	McGowan Method
pc	2749.78	kPa	Joback Method
tb	624.30	K	Joback Method
tc	817.10	K	Joback Method
tf	355.47	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.83	J/molxK	624.30	Joback Method
cpg	465.32	J/molxK	784.97	Joback Method
cpg	455.04	J/molxK	752.83	Joback Method
cpg	444.14	J/molxK	720.70	Joback Method
cpg	432.64	J/molxK	688.57	Joback Method
cpg	420.54	J/molxK	656.43	Joback Method
cpg	475.00	J/molxK	817.10	Joback Method
dvisc	0.0000437	Paxs	624.30	Joback Method
dvisc	0.0000655	Paxs	579.49	Joback Method

dvisc	0.0001053	Paxs	534.69	Joback Method
dvisc	0.0001845	Paxs	489.88	Joback Method
dvisc	0.0003619	Paxs	445.08	Joback Method
dvisc	0.0008255	Paxs	400.28	Joback Method
dvisc	0.0023179	Paxs	355.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40180969&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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