R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenon (desmethyl-3-methoxy-desamino-oxo-), ethylated

Other names:	R,S-3',4'-methylenedioxy-«alpha»-pyrrolidinopropiophenone-M (desmethylene-3-methyl-desamino-oxo-), ethylated
Inchi:	InChI=1S/C12H14O4/c1-4-16-10-6-5-9(7-11(10)15-3)12(14)8(2)13/h5-7H,4H2,1-3H3
InchiKey:	PFGFBGCGXNIEJR-UHFFFAOYSA-N
Formula:	C12H14O4
SMILES:	CCOc1ccc(C(=O)C(C)=O)cc1OC
Mol. weight [g/mol]:	222.24

Physical Properties

Property code	Value	Unit	Source
gf	-324.53	kJ/mol	Joback Method
hf	-567.02	kJ/mol	Joback Method
hfus	25.67	kJ/mol	Joback Method
hvap	64.22	kJ/mol	Joback Method
log10ws	-2.49		Crippen Method
logp	1.866		Crippen Method
mcvol	171.060	ml/mol	McGowan Method
pc	2558.51	kPa	Joback Method
rinpol	1680.00		NIST Webbook
rinpol	1680.00		NIST Webbook
tb	663.18	K	Joback Method
tc	875.86	K	Joback Method
tf	420.78	K	Joback Method
vc	0.647	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.52	J/mol×K	663.18	Joback Method
cpg	448.70	J/mol×K	698.63	Joback Method
cpg	461.11	J/mol×K	734.07	Joback Method
cpg	472.74	J/mol×K	769.52	Joback Method
cpg	483.58	J/mol×K	804.97	Joback Method
cpg	493.62	J/mol×K	840.42	Joback Method
cpg	502.86	J/mol×K	875.86	Joback Method

dvisc	0.0009239	Pa×s	420.78	Joback Method
dvisc	0.0005957	Pa×s	461.18	Joback Method
dvisc	0.0004122	Pa×s	501.58	Joback Method
dvisc	0.0003014	Pa×s	541.98	Joback Method
dvisc	0.0002301	Pa×s	582.38	Joback Method
dvisc	0.0001820	Pa×s	622.78	Joback Method
dvisc	0.0001481	Pa×s	663.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R290625&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume