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

InChI: InChI=1S/C11H12O3/c1-3-14-10-6-4-9(5-7-10)11(13)8(2)12/h4-7H,3H2,1-2H3
InChIKey: SETGTABDCSJQPU-UHFFFAOYSA-N
Formula: C11H12O3
SMILES: CCOc1ccc(C(=O)C(C)=O)cc1
Mol. weight [g/mol]: 192.21

Physical Properties

Property code	Value	Unit	Source
gf	-218.32	kJ/mol	Joback Method
hf	-402.69	kJ/mol	Joback Method
hfus	22.28	kJ/mol	Joback Method
hvap	58.92	kJ/mol	Joback Method
log10ws	-2.37		Crippen Method
logp	1.857		Crippen Method
mcvol	151.100	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	1530.00		NIST Webbook
tb	612.90	K	Joback Method
tc	830.79	K	Joback Method
tf	374.76	K	Joback Method
vc	0.574	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	362.73	J/mol×K	612.90	Joback Method
cpg	375.63	J/mol×K	649.21	Joback Method
cpg	387.75	J/mol×K	685.53	Joback Method
cpg	399.09	J/mol×K	721.84	Joback Method
cpg	409.67	J/mol×K	758.16	Joback Method
cpg	419.51	J/mol×K	794.47	Joback Method
cpg	428.62	J/mol×K	830.79	Joback Method
dvisc	0.0015551	Pa×s	374.76	Joback Method
dvisc	0.0009466	Pa×s	414.45	Joback Method

dvisc	0.0006284	Pa×s	454.14	Joback Method
dvisc	0.0004456	Pa×s	493.83	Joback Method
dvisc	0.0003325	Pa×s	533.52	Joback Method
dvisc	0.0002584	Pa×s	573.21	Joback Method
dvisc	0.0002075	Pa×s	612.90	Joback Method

Sources

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=R290630&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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