

R,S-4'-Methoxy-«alpha»-pyrrolidinopropiophenone

InChI: InChI=1S/C10H10O3/c1-7(11)10(12)8-3-5-9(13-2)6-4-8/h3-6H,1-2H3
(desamino-oxo-)
InChIKey: YOJWSQBCJZWMIR-UHFFFAOYSA-N

Formula: C10H10O3
SMILES: COc1ccc(C(=O)C(C)=O)cc1
Mol. weight [g/mol]: 178.18

Physical Properties

Property code	Value	Unit	Source
gf	-226.74	kJ/mol	Joback Method
hf	-382.05	kJ/mol	Joback Method
hfus	19.69	kJ/mol	Joback Method
hvap	56.69	kJ/mol	Joback Method
log10ws	-1.95		Crippen Method
logp	1.467		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3254.14	kPa	Joback Method
rinpol	1440.00		NIST Webbook
rinpol	1440.00		NIST Webbook
tb	590.02	K	Joback Method
tc	811.87	K	Joback Method
tf	363.49	K	Joback Method
vc	0.517	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	315.55	J/molxK	590.02	Joback Method
cpg	327.63	J/molxK	626.99	Joback Method
cpg	338.98	J/molxK	663.97	Joback Method
cpg	349.60	J/molxK	700.94	Joback Method
cpg	359.51	J/molxK	737.92	Joback Method
cpg	368.72	J/molxK	774.89	Joback Method
cpg	377.23	J/molxK	811.87	Joback Method
dvisc	0.0015944	Paxs	363.49	Joback Method

dvisc	0.0009880	Paxs	401.25	Joback Method
dvisc	0.0006648	Paxs	439.00	Joback Method
dvisc	0.0004763	Paxs	476.75	Joback Method
dvisc	0.0003583	Paxs	514.51	Joback Method
dvisc	0.0002803	Paxs	552.26	Joback Method
dvisc	0.0002262	Paxs	590.02	Joback Method

Sources

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=R290576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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