1-(3,4-Dimethoxyphenyl)pentan-3-one

Inchi: InChI=1S/C13H18O3/c1-4-11(14)7-5-10-6-8-12(15-2)13(9-10)16-3/h6,8-9H,4-5,7H2,1-3H
InchiKey: SOWKMIKWOOVRAB-UHFFFAOYSA-N
Formula: C13H18O3
SMILES: CCC(=O)CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 222.28
CAS: 39728-56-8

Physical Properties

Property code	Value	Unit	Source
gf	-187.19	kJ/mol	Joback Method
hf	-475.08	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	59.70	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.615		Crippen Method
mcvol	183.580	ml/mol	McGowan Method
pc	2191.78	kPa	Joback Method
rinpol	1786.50		NIST Webbook
rinpol	1786.50		NIST Webbook
tb	632.19	K	Joback Method
tc	835.04	K	Joback Method
tf	382.12	K	Joback Method
vc	0.698	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	468.92	J/mol×K	632.19	Joback Method
cpg	536.60	J/mol×K	801.23	Joback Method
cpg	524.61	J/mol×K	767.43	Joback Method
cpg	511.85	J/mol×K	733.62	Joback Method
cpg	498.32	J/mol×K	699.81	Joback Method
cpg	484.01	J/mol×K	666.00	Joback Method
cpg	547.81	J/mol×K	835.04	Joback Method

dvisc	0.0001297	Pa×s	632.19	Joback Method
dvisc	0.0001613	Pa×s	590.51	Joback Method
dvisc	0.0002075	Pa×s	548.83	Joback Method
dvisc	0.0002781	Pa×s	507.16	Joback Method
dvisc	0.0003927	Pa×s	465.48	Joback Method
dvisc	0.0005937	Pa×s	423.80	Joback Method
dvisc	0.0009821	Pa×s	382.12	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39728568&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

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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