

1-(3,4-Dimethoxyphenyl)-5-methoxydecan-3-one

Inchi:	InChI=1S/C19H30O4/c1-5-6-7-8-17(21-2)14-16(20)11-9-15-10-12-18(22-3)19(13-15)23-4
InchiKey:	IZEIPXBCPYUZCX-UHFFFAOYSA-N
Formula:	C19H30O4
SMILES:	CCCCC(CC(=O)CCc1ccc(OC)c(OC)c1)OC
Mol. weight [g/mol]:	322.44

Physical Properties

Property code	Value	Unit	Source
gf	-244.11	kJ/mol	Joback Method
hf	-736.42	kJ/mol	Joback Method
hfus	39.87	kJ/mol	Joback Method
hvap	75.08	kJ/mol	Joback Method
log10ws	-4.76		Crippen Method
logp	4.191		Crippen Method
mvol	273.990	ml/mol	McGowan Method
pc	1350.65	kPa	Joback Method
rinpol	2375.10		NIST Webbook
rinpol	2375.10		NIST Webbook
tb	791.45	K	Joback Method
tc	986.79	K	Joback Method
tf	456.97	K	Joback Method
vc	1.046	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	828.42	J/molxK	791.45	Joback Method
cpg	845.66	J/molxK	824.01	Joback Method
cpg	861.82	J/molxK	856.56	Joback Method
cpg	876.87	J/molxK	889.12	Joback Method
cpg	890.84	J/molxK	921.68	Joback Method
cpg	903.73	J/molxK	954.23	Joback Method
cpg	915.53	J/molxK	986.79	Joback Method
dvisc	0.0005422	Paxs	456.97	Joback Method

dvisc	0.0002865	Paxs	512.72	Joback Method
dvisc	0.0001716	Paxs	568.46	Joback Method
dvisc	0.0001126	Paxs	624.21	Joback Method
dvisc	0.0000792	Paxs	679.96	Joback Method
dvisc	0.0000587	Paxs	735.70	Joback Method
dvisc	0.0000454	Paxs	791.45	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=U412832&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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