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

Inchi: InChI=1S/C18H28O3/c1-4-5-6-7-8-9-16(19)12-10-15-11-13-17(20-2)18(14-15)21-3/h11,1
InchiKey: WPGKEQMMTRTWDF-UHFFFAOYSA-N
Formula: C18H28O3
SMILES: CCCCCCCC(=O)CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 292.41
CAS: 39728-61-5

Physical Properties

Property code	Value	Unit	Source
gf	-145.09	kJ/mol	Joback Method
hf	-578.28	kJ/mol	Joback Method
hfus	39.61	kJ/mol	Joback Method
hvap	70.83	kJ/mol	Joback Method
log10ws	-5.14		Crippen Method
logp	4.566		Crippen Method
mcvol	254.030	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	2267.90		NIST Webbook
rinpol	2267.90		NIST Webbook
tb	746.59	K	Joback Method
tc	939.89	K	Joback Method
tf	438.47	K	Joback Method
vc	0.978	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	740.07	J/mol×K	746.59	Joback Method
cpg	816.28	J/mol×K	907.67	Joback Method
cpg	802.95	J/mol×K	875.46	Joback Method
cpg	788.67	J/mol×K	843.24	Joback Method
cpg	773.44	J/mol×K	811.02	Joback Method
cpg	757.25	J/mol×K	778.81	Joback Method
cpg	828.68	J/mol×K	939.89	Joback Method

dvisc	0.0000738	Pa×s	746.59	Joback Method
dvisc	0.0000938	Pa×s	695.24	Joback Method
dvisc	0.0001239	Pa×s	643.88	Joback Method
dvisc	0.0001717	Pa×s	592.53	Joback Method
dvisc	0.0002533	Pa×s	541.18	Joback Method
dvisc	0.0004053	Pa×s	489.82	Joback Method
dvisc	0.0007241	Pa×s	438.47	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39728615&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