

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
mvol	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	m ³ /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	Paxs	746.59	Joback Method
dvisc	0.0000938	Paxs	695.24	Joback Method
dvisc	0.0001239	Paxs	643.88	Joback Method
dvisc	0.0001717	Paxs	592.53	Joback Method
dvisc	0.0002533	Paxs	541.18	Joback Method
dvisc	0.0004053	Paxs	489.82	Joback Method
dvisc	0.0007241	Paxs	438.47	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=C39728615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
mvol:	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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