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

Inchi: InChI=1S/C15H22O3/c1-4-5-6-13(16)9-7-12-8-10-14(17-2)15(11-12)18-3/h8,10-11H,4-7,
InchiKey: OWMYBRGRNJCGGA-UHFFFAOYSA-N
Formula: C15H22O3
SMILES: CCCCC(=O)CCc1ccc(OC)c(OC)c1
Mol. weight [g/mol]: 250.33
CAS: 39728-58-0

Physical Properties

Property code	Value	Unit	Source
gf	-170.35	kJ/mol	Joback Method
hf	-516.36	kJ/mol	Joback Method
hfus	31.84	kJ/mol	Joback Method
hvap	64.15	kJ/mol	Joback Method
log10ws	-3.89		Crippen Method
logp	3.396		Crippen Method
mcvol	211.760	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1863.20		NIST Webbook
rinpol	1863.20		NIST Webbook
tb	677.95	K	Joback Method
tc	875.77	K	Joback Method
tf	404.66	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	573.56	J/mol×K	677.95	Joback Method
cpg	589.67	J/mol×K	710.92	Joback Method
cpg	604.92	J/mol×K	743.89	Joback Method
cpg	619.31	J/mol×K	776.86	Joback Method
cpg	632.86	J/mol×K	809.83	Joback Method
cpg	645.55	J/mol×K	842.80	Joback Method
cpg	657.41	J/mol×K	875.77	Joback Method

dvisc	0.0008897	Pa×s	404.66	Joback Method
dvisc	0.0005205	Pa×s	450.21	Joback Method
dvisc	0.0003360	Pa×s	495.76	Joback Method
dvisc	0.0002335	Pa×s	541.31	Joback Method
dvisc	0.0001717	Pa×s	586.85	Joback Method
dvisc	0.0001320	Pa×s	632.40	Joback Method
dvisc	0.0001051	Pa×s	677.95	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C39728580&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