Octanoic acid, 6,6-dimethoxy-, methyl ester

Inchi: InChI=1S/C11H22O4/c1-13-10(12)8-6-4-5-7-9-11(14-2)15-3/h11H,4-9H2,1-3H3
InchiKey: BYAKBTBKBLTLPV-UHFFFAOYSA-N
Formula: C11H22O4
SMILES: COC(=O)CCCCCCC(OC)OC
Mol. weight [g/mol]: 218.29
CAS: 65157-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-404.62	kJ/mol	Joback Method
hf	-784.89	kJ/mol	Joback Method
hfus	25.89	kJ/mol	Joback Method
hvap	53.67	kJ/mol	Joback Method
log10ws	-2.07		Crippen Method
logp	2.119		Crippen Method
mcvol	185.030	ml/mol	McGowan Method
pc	1968.30	kPa	Joback Method
rinpol	1601.00		NIST Webbook
tb	571.77	K	Joback Method
tc	744.96	K	Joback Method
tf	315.35	K	Joback Method
vc	0.706	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	469.67	J/mol×K	571.77	Joback Method
cpg	484.57	J/mol×K	600.63	Joback Method
cpg	498.93	J/mol×K	629.50	Joback Method
cpg	512.74	J/mol×K	658.36	Joback Method
cpg	526.00	J/mol×K	687.23	Joback Method
cpg	538.69	J/mol×K	716.09	Joback Method
cpg	550.81	J/mol×K	744.96	Joback Method
dvisc	0.0021183	Pa×s	315.35	Joback Method

dvisc	0.0009950	Pa×s	358.09	Joback Method
dvisc	0.0005491	Pa×s	400.82	Joback Method
dvisc	0.0003398	Pa×s	443.56	Joback Method
dvisc	0.0002288	Pa×s	486.30	Joback Method
dvisc	0.0001642	Pa×s	529.03	Joback Method
dvisc	0.0001239	Pa×s	571.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C65157893&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