Oct-3-enoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C16H28O2/c1-4-6-8-10-12-14-16(17)18-15(3)13-11-9-7-5-2/h10-13,15H,4-9,14
InchiKey: DHMLVAHJCQWZQK-DCIPZJNNSA-N
Formula: C16H28O2
SMILES: CCCCC=CCC(=O)OC(C)C=CCCCC
Mol. weight [g/mol]: 252.39

Physical Properties

Property code	Value	Unit	Source
gf	7.92	kJ/mol	Joback Method
hf	-389.21	kJ/mol	Joback Method
hfus	36.86	kJ/mol	Joback Method
hvap	59.89	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	4.801		Crippen Method
mcvol	235.140	ml/mol	McGowan Method
pc	1483.85	kPa	Joback Method
rinpol	1688.00		NIST Webbook
rinpol	1688.00		NIST Webbook
tb	649.65	K	Joback Method
tc	830.18	K	Joback Method
tf	317.08	K	Joback Method
vc	0.909	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	634.54	J/mol×K	649.65	Joback Method
cpg	651.88	J/mol×K	679.74	Joback Method
cpg	668.39	J/mol×K	709.83	Joback Method
cpg	684.10	J/mol×K	739.91	Joback Method
cpg	699.05	J/mol×K	770.00	Joback Method
cpg	713.26	J/mol×K	800.09	Joback Method
cpg	726.78	J/mol×K	830.18	Joback Method
dvisc	0.0028040	Pa×s	317.08	Joback Method

dvisc	0.0010102	Pa×s	372.51	Joback Method
dvisc	0.0004741	Pa×s	427.94	Joback Method
dvisc	0.0002647	Pa×s	483.37	Joback Method
dvisc	0.0001666	Pa×s	538.79	Joback Method
dvisc	0.0001143	Pa×s	594.22	Joback Method
dvisc	0.0000836	Pa×s	649.65	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U406950&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

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