2-Heptenoic acid, oct-3-en-2-yl ester

Inchi: InChI=1S/C15H26O2/c1-4-6-8-10-12-14(3)17-15(16)13-11-9-7-5-2/h10-14H,4-9H2,1-3H3
InchiKey: ZRGIQNZDTIXKDU-DCIPZJNNSA-N
Formula: C15H26O2
SMILES: CCCCC=CC(=O)OC(C)C=CCCCC
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	-0.50	kJ/mol	Joback Method
hf	-368.57	kJ/mol	Joback Method
hfus	34.27	kJ/mol	Joback Method
hvap	57.67	kJ/mol	Joback Method
log10ws	-4.78		Crippen Method
logp	4.411		Crippen Method
mcvol	221.050	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpol	2113.00		NIST Webbook
tb	626.77	K	Joback Method
tc	808.54	K	Joback Method
tf	305.81	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.58	J/mol×K	626.77	Joback Method
cpg	657.33	J/mol×K	778.24	Joback Method
cpg	643.47	J/mol×K	747.95	Joback Method
cpg	628.91	J/mol×K	717.65	Joback Method
cpg	613.59	J/mol×K	687.36	Joback Method
cpg	597.49	J/mol×K	657.06	Joback Method
cpg	670.50	J/mol×K	808.54	Joback Method
dvisc	0.0000937	Pa×s	626.77	Joback Method
dvisc	0.0001278	Pa×s	573.28	Joback Method

dvisc	0.0001856	Pa×s	519.78	Joback Method
dvisc	0.0002939	Pa×s	466.29	Joback Method
dvisc	0.0005240	Pa×s	412.80	Joback Method
dvisc	0.0011102	Pa×s	359.30	Joback Method
dvisc	0.0030582	Pa×s	305.81	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=U406942&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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