

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

Inchi:	InChI=1S/C16H30O2/c1-4-6-8-10-12-14-16(17)18-15(3)13-11-9-7-5-2/h11,13,15H,4-10,1
InchiKey:	YLCXQAGJQBBVIX-ACCUITESSA-N
Formula:	C16H30O2
SMILES:	CCCCC=CC(C)OC(=O)CCCCCCC
Mol. weight [g/mol]:	254.41

Physical Properties

Property code	Value	Unit	Source
gf	-72.30	kJ/mol	Joback Method
hf	-506.43	kJ/mol	Joback Method
hfus	36.66	kJ/mol	Joback Method
hvap	59.94	kJ/mol	Joback Method
log10ws	-5.35		Crippen Method
logp	5.025		Crippen Method
mvol	239.440	ml/mol	McGowan Method
pc	1426.15	kPa	Joback Method
rinpol	1666.00		NIST Webbook
tb	645.49	K	Joback Method
tc	820.35	K	Joback Method
tf	322.16	K	Joback Method
vc	0.929	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	655.51	J/mol×K	645.49	Joback Method
cpg	673.27	J/mol×K	674.63	Joback Method
cpg	690.23	J/mol×K	703.78	Joback Method
cpg	706.40	J/mol×K	732.92	Joback Method
cpg	721.81	J/mol×K	762.07	Joback Method
cpg	736.48	J/mol×K	791.21	Joback Method
cpg	750.45	J/mol×K	820.35	Joback Method
dvisc	0.0029760	Paxs	322.16	Joback Method
dvisc	0.0011188	Paxs	376.05	Joback Method

dvisc	0.0005375	Paxs	429.94	Joback Method
dvisc	0.0003041	Paxs	483.82	Joback Method
dvisc	0.0001928	Paxs	537.71	Joback Method
dvisc	0.0001328	Paxs	591.60	Joback Method
dvisc	0.0000974	Paxs	645.49	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U299344&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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