m-Toluic acid, oct-3-en-2-yl ester

Other names: m-toluylic acid, oct-3-en-2-yl ester
Inchi: InChI=1S/C16H22O2/c1-4-5-6-7-10-14(3)18-16(17)15-11-8-9-13(2)12-15/h7-12,14H,4-6H
InchiKey: LZHUDNPJQUBRGF-JXMROGBWSA-N
Formula: C16H22O2
SMILES: CCCCC=CC(C)OC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 246.34

Physical Properties

Property code	Value	Unit	Source
gf	30.48	kJ/mol	Joback Method
hf	-281.37	kJ/mol	Joback Method
hfus	30.31	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-5.09		Crippen Method
logp	4.287		Crippen Method
mcvol	215.680	ml/mol	McGowan Method
pc	1838.84	kPa	Joback Method
rinpol	1797.40		NIST Webbook
rinpol	1797.40		NIST Webbook
tb	677.15	K	Joback Method
tc	883.85	K	Joback Method
tf	361.10	K	Joback Method
vc	0.822	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	578.07	J/mol×K	677.15	Joback Method
cpg	594.92	J/mol×K	711.60	Joback Method
cpg	610.77	J/mol×K	746.05	Joback Method
cpg	625.67	J/mol×K	780.50	Joback Method
cpg	639.64	J/mol×K	814.95	Joback Method
cpg	652.74	J/mol×K	849.40	Joback Method
cpg	665.00	J/mol×K	883.85	Joback Method

dvisc	0.0016206	Pa×s	361.10	Joback Method
dvisc	0.0007510	Pa×s	413.78	Joback Method
dvisc	0.0004141	Pa×s	466.45	Joback Method
dvisc	0.0002576	Pa×s	519.12	Joback Method
dvisc	0.0001749	Pa×s	571.80	Joback Method
dvisc	0.0001268	Pa×s	624.48	Joback Method
dvisc	0.0000966	Pa×s	677.15	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292612&Units=SI

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