o-Toluic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester

Other names: o-toluylic acid, 2,7-dimethyloct-7-en-5-yn-4-yl ester
Inchi: InChI=1S/C18H22O2/c1-13(2)10-11-16(12-14(3)4)20-18(19)17-9-7-6-8-15(17)5/h6-9,14,
InchiKey: FJIDCSVODBXXTA-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: C=C(C)C#CC(CC(C)C)OC(=O)c1ccccc1C
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
gf	246.75	kJ/mol	Joback Method
hf	-57.21	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	68.54	kJ/mol	Joback Method
log10ws	-5.48		Crippen Method
logp	4.146		Crippen Method
mcvol	235.260	ml/mol	McGowan Method
pc	1793.94	kPa	Joback Method
rinpol	1857.70		NIST Webbook
tb	723.87	K	Joback Method
tc	948.28	K	Joback Method
tf	464.10	K	Joback Method
vc	0.891	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.06	J/mol×K	723.87	Joback Method
cpg	658.62	J/mol×K	761.27	Joback Method
cpg	675.02	J/mol×K	798.67	Joback Method
cpg	690.30	J/mol×K	836.07	Joback Method
cpg	704.50	J/mol×K	873.47	Joback Method
cpg	717.66	J/mol×K	910.88	Joback Method
cpg	729.82	J/mol×K	948.28	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292515&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
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