m-Toluic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester

Other names: m-toluylic acid, 2,6-dimethylnon-1-en-3-yn-5-yl ester
Inchi: InChI=1S/C19H24O2/c1-6-8-16(5)18(12-11-14(2)3)21-19(20)17-10-7-9-15(4)13-17/h7,9-
InchiKey: FPLHZSOEGPVHMS-UHFFFAOYSA-N
Formula: C19H24O2
SMILES: C=C(C)C#CC(OC(=O)c1cccc(C)c1)C(C)CCC
Mol. weight [g/mol]: 284.39

Physical Properties

Property code	Value	Unit	Source
gf	255.17	kJ/mol	Joback Method
hf	-77.85	kJ/mol	Joback Method
hfus	34.89	kJ/mol	Joback Method
hvap	70.77	kJ/mol	Joback Method
log10ws	-5.89		Crippen Method
logp	4.536		Crippen Method
mcvol	249.350	ml/mol	McGowan Method
pc	1656.49	kPa	Joback Method
rinpol	1962.40		NIST Webbook
tb	746.75	K	Joback Method
tc	967.62	K	Joback Method
tf	475.37	K	Joback Method
vc	0.948	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	696.60	J/mol×K	746.75	Joback Method
cpg	714.39	J/mol×K	783.56	Joback Method
cpg	731.01	J/mol×K	820.37	Joback Method
cpg	746.49	J/mol×K	857.19	Joback Method
cpg	760.89	J/mol×K	894.00	Joback Method
cpg	774.24	J/mol×K	930.81	Joback Method
cpg	786.60	J/mol×K	967.62	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=U292498&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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