m-Toluic acid, hex-4-yn-3-yl ester

Other names: m-toluylic acid, hex-4-yn-3-yl ester
Inchi: InChI=1S/C14H16O2/c1-4-7-13(5-2)16-14(15)12-9-6-8-11(3)10-12/h6,8-10,13H,5H2,1-3H
InchiKey: OANBDRKPBKUOIH-UHFFFAOYSA-N
Formula: C14H16O2
SMILES: CC#CC(CC)OC(=O)c1cccc(C)c1
Mol. weight [g/mol]: 216.28

Physical Properties

Property code	Value	Unit	Source
gf	136.22	kJ/mol	Joback Method
hf	-85.01	kJ/mol	Joback Method
hfus	28.05	kJ/mol	Joback Method
hvap	60.62	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	2.954		Crippen Method
mcvol	183.200	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1667.60		NIST Webbook
rinpol	1667.60		NIST Webbook
tb	636.23	K	Joback Method
tc	864.73	K	Joback Method
tf	449.74	K	Joback Method
vc	0.692	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	452.85	J/mol×K	636.23	Joback Method
cpg	468.77	J/mol×K	674.31	Joback Method
cpg	483.70	J/mol×K	712.40	Joback Method
cpg	497.67	J/mol×K	750.48	Joback Method
cpg	510.69	J/mol×K	788.57	Joback Method
cpg	522.80	J/mol×K	826.65	Joback Method
cpg	534.01	J/mol×K	864.73	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=U292496&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