o-Toluic acid, 2-methyloct-5-yn-4-yl ester

Other names: o-toluylic acid, 2-methyloct-5-yn-4-yl ester
Inchi: InChI=1S/C17H22O2/c1-5-6-10-15(12-13(2)3)19-17(18)16-11-8-7-9-14(16)4/h7-9,11,13,1
InchiKey: KSYYDHHACWSADT-UHFFFAOYSA-N
Formula: C17H22O2
SMILES: CCC#CC(CC(C)C)OC(=O)c1ccccc1C
Mol. weight [g/mol]: 258.36

Physical Properties

Property code	Value	Unit	Source
gf	159.04	kJ/mol	Joback Method
hf	-152.21	kJ/mol	Joback Method
hfus	32.30	kJ/mol	Joback Method
hvap	66.91	kJ/mol	Joback Method
log10ws	-5.20		Crippen Method
logp	3.980		Crippen Method
mcvol	225.470	ml/mol	McGowan Method
pc	1870.79	kPa	Joback Method
rinpol	1809.30		NIST Webbook
rinpol	1809.30		NIST Webbook
tb	704.43	K	Joback Method
tc	925.13	K	Joback Method
tf	468.55	K	Joback Method
vc	0.854	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	610.91	J/mol×K	704.43	Joback Method
cpg	628.49	J/mol×K	741.21	Joback Method
cpg	644.95	J/mol×K	778.00	Joback Method
cpg	660.32	J/mol×K	814.78	Joback Method
cpg	674.63	J/mol×K	851.56	Joback Method
cpg	687.92	J/mol×K	888.35	Joback Method
cpg	700.21	J/mol×K	925.13	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=U292514&Units=SI

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