

o-Toluic acid, tridec-2-ynyl ester

Other names:	o-toluylic acid, tridec-2-ynyl ester
Inchi:	InChI=1S/C21H30O2/c1-3-4-5-6-7-8-9-10-11-12-15-18-23-21(22)20-17-14-13-16-19(20)
InchiKey:	MZZHYTYNGJPMNW-UHFFFAOYSA-N
Formula:	C21H30O2
SMILES:	CCCCCCCCCCC#CCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	314.46

Physical Properties

Property code	Value	Unit	Source
gf	197.60	kJ/mol	Joback Method
hf	-224.21	kJ/mol	Joback Method
hfus	49.71	kJ/mol	Joback Method
hvap	76.59	kJ/mol	Joback Method
log10ws	-7.01		Crippen Method
logp	5.686		Crippen Method
mcvol	281.830	ml/mol	McGowan Method
pc	1359.63	kPa	Joback Method
rinpol	2400.90		NIST Webbook
tb	796.83	K	Joback Method
tc	1001.35	K	Joback Method
tf	543.63	K	Joback Method
vc	1.089	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	836.53	J/molxK	796.83	Joback Method
cpg	854.43	J/molxK	830.92	Joback Method
cpg	871.22	J/molxK	865.00	Joback Method
cpg	886.94	J/molxK	899.09	Joback Method
cpg	901.63	J/molxK	933.18	Joback Method
cpg	915.32	J/molxK	967.27	Joback Method
cpg	928.06	J/molxK	1001.35	Joback Method

Sources

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=U292517&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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