

o-Toluic acid, dodec-9-ynyl ester

Other names:	o-toluylic acid, dodec-9-ynyl ester
Inchi:	InChI=1S/C20H28O2/c1-3-4-5-6-7-8-9-10-11-14-17-22-20(21)19-16-13-12-15-18(19)2/h1
InchiKey:	GOLJVAJTVIMORZ-UHFFFAOYSA-N
Formula:	C20H28O2
SMILES:	CCC#CCCCCCCCCOC(=O)c1ccccc1C
Mol. weight [g/mol]:	300.44

Physical Properties

Property code	Value	Unit	Source
gf	189.18	kJ/mol	Joback Method
hf	-203.57	kJ/mol	Joback Method
hfus	47.12	kJ/mol	Joback Method
hvap	74.36	kJ/mol	Joback Method
log10ws	-6.59		Crippen Method
logp	5.296		Crippen Method
mcvol	267.740	ml/mol	McGowan Method
pc	1461.25	kPa	Joback Method
rinpol	2321.00		NIST Webbook
rinpol	2321.00		NIST Webbook
tb	773.95	K	Joback Method
tc	979.79	K	Joback Method
tf	532.36	K	Joback Method
vc	1.034	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	778.34	J/molxK	773.95	Joback Method
cpg	796.04	J/molxK	808.26	Joback Method
cpg	812.66	J/molxK	842.56	Joback Method
cpg	828.23	J/molxK	876.87	Joback Method
cpg	842.78	J/molxK	911.18	Joback Method
cpg	856.35	J/molxK	945.49	Joback Method
cpg	868.97	J/molxK	979.79	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292229&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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

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