p-Toluic acid, 3-methylbut-2-enyl ester

Other names:	p-Toluylic acid, 3-methylbut-2-enyl ester
Inchi:	InChI=1S/C13H16O2/c1-10(2)8-9-15-13(14)12-6-4-11(3)5-7-12/h4-8H,9H2,1-3H3
InchiKey:	DTWKHCCYFGKBMV-UHFFFAOYSA-N
Formula:	C13H16O2
SMILES:	CC(C)=CCOC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	204.26
CAS:	154559-35-0

Physical Properties

Property code	Value	Unit	Source
gf	-0.89	kJ/mol	Joback Method
hf	-223.96	kJ/mol	Joback Method
hfus	24.76	kJ/mol	Joback Method
hvap	56.66	kJ/mol	Joback Method
log10ws	-3.72		Crippen Method
logp	3.118		Crippen Method
mcvol	173.410	ml/mol	McGowan Method
pc	2386.52	kPa	Joback Method
rinpol	1622.80		NIST Webbook
tb	608.83	K	Joback Method
tc	824.83	K	Joback Method
tf	328.33	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.38	J/mol×K	608.83	Joback Method
cpg	437.67	J/mol×K	644.83	Joback Method
cpg	452.04	J/mol×K	680.83	Joback Method
cpg	465.53	J/mol×K	716.83	Joback Method
cpg	478.17	J/mol×K	752.83	Joback Method
cpg	490.01	J/mol×K	788.83	Joback Method
cpg	501.08	J/mol×K	824.83	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=C154559350&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

Latest version available from:

https://www.chemeo.com/cid/45-996-7/p-Toluic-acid-3-methylbut-2-enyl-ester.pdf

Generated by Cheméo on 2024-10-12 07:19:47.39649093 +0000 UTC m=+3298450.033460178.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.