p-Toluic acid, 2-adamantyl ester

Other names: p-toluylic acid, 2-adamantyl ester
Inchi: InChI=1S/C18H22O2/c1-11-2-4-14(5-3-11)18(19)20-17-15-7-12-6-13(9-15)10-16(17)8-12
InchiKey: LIZCHCUUPZQFIY-UHFFFAOYSA-N
Formula: C18H22O2
SMILES: Cc1ccc(C(=O)OC2C3CC4CC(C3)CC2C4)cc1
Mol. weight [g/mol]: 270.37

Physical Properties

Property code	Value	Unit	Source
gf	124.27	kJ/mol	Joback Method
hf	-263.03	kJ/mol	Joback Method
hfus	33.26	kJ/mol	Joback Method
hvap	67.05	kJ/mol	Joback Method
log10ws	-4.79		Crippen Method
logp	3.977		Crippen Method
mcvol	215.580	ml/mol	McGowan Method
pc	2001.91	kPa	Joback Method
rinpol	2215.70		NIST Webbook
rinpol	2215.70		NIST Webbook
tb	734.34	K	Joback Method
tc	967.98	K	Joback Method
tf	445.54	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	673.94	J/mol×K	734.34	Joback Method
cpg	762.64	J/mol×K	929.04	Joback Method
cpg	747.30	J/mol×K	890.10	Joback Method
cpg	730.89	J/mol×K	851.16	Joback Method
cpg	713.27	J/mol×K	812.22	Joback Method
cpg	694.33	J/mol×K	773.28	Joback Method
cpg	777.03	J/mol×K	967.98	Joback Method

dvisc	0.0023353	Pa×s	734.34	Joback Method
dvisc	0.0024557	Pa×s	686.21	Joback Method
dvisc	0.0026020	Pa×s	638.07	Joback Method
dvisc	0.0027831	Pa×s	589.94	Joback Method
dvisc	0.0030126	Pa×s	541.81	Joback Method
dvisc	0.0033118	Pa×s	493.67	Joback Method
dvisc	0.0037160	Pa×s	445.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292216&Units=SI
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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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