

m-Toluic acid, 2-adamantyl ester

Other names:	m-toluylic acid, 2-adamantyl ester
Inchi:	InChI=1S/C18H22O2/c1-11-3-2-4-14(5-11)18(19)20-17-15-7-12-6-13(9-15)10-16(17)8-12
InchiKey:	SNPNELJYAGDMFC-UHFFFAOYSA-N
Formula:	C18H22O2
SMILES:	<chem>Cc1cccc(C(=O)OC2C3CC4CC(C3)CC2C4)c1</chem>
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	2211.20		NIST Webbook
rinpol	2211.20		NIST Webbook
tb	734.34	K	Joback Method
tc	967.98	K	Joback Method
tf	445.54	K	Joback Method
vc	0.821	m ³ /kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0037160	Paxs	445.54	Joback Method
dvisc	0.0033118	Paxs	493.67	Joback Method
dvisc	0.0030126	Paxs	541.81	Joback Method
dvisc	0.0027831	Paxs	589.94	Joback Method
dvisc	0.0026020	Paxs	638.07	Joback Method
dvisc	0.0024557	Paxs	686.21	Joback Method
dvisc	0.0023353	Paxs	734.34	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=U292234&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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