

o-Anisic acid, 2-adamantyl ester

Inchi:	InChI=1S/C18H22O3/c1-20-16-5-3-2-4-15(16)18(19)21-17-13-7-11-6-12(9-13)10-14(17)8
InchiKey:	KWHKSGIIGZCYIR-UHFFFAOYSA-N
Formula:	C18H22O3
SMILES:	COc1ccccc1C(=O)OC1C2CC3CC(C2)CC1C3
Mol. weight [g/mol]:	286.37

Physical Properties

Property code	Value	Unit	Source
gf	19.27	kJ/mol	Joback Method
hf	-395.25	kJ/mol	Joback Method
hfus	34.45	kJ/mol	Joback Method
hvap	69.46	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	3.677		Crippen Method
mvol	221.450	ml/mol	McGowan Method
pc	1971.80	kPa	Joback Method
rinpol	2313.00		NIST Webbook
tb	756.76	K	Joback Method
tc	987.36	K	Joback Method
tf	467.77	K	Joback Method
vc	0.839	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.35	J/molxK	756.76	Joback Method
cpg	788.75	J/molxK	948.92	Joback Method
cpg	774.07	J/molxK	910.49	Joback Method
cpg	758.30	J/molxK	872.06	Joback Method
cpg	741.32	J/molxK	833.63	Joback Method
cpg	723.04	J/molxK	795.19	Joback Method
cpg	802.43	J/molxK	987.36	Joback Method
dvisc	0.0019343	Paxs	756.76	Joback Method
dvisc	0.0020503	Paxs	708.60	Joback Method

dvisc	0.0021918	Paxs	660.43	Joback Method
dvisc	0.0023677	Paxs	612.27	Joback Method
dvisc	0.0025918	Paxs	564.10	Joback Method
dvisc	0.0028853	Paxs	515.93	Joback Method
dvisc	0.0032839	Paxs	467.77	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=U299948&Units=SI

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

Latest version available from:

<https://www.chemeo.com/cid/50-755-8/o-Anisic-acid-2-adamantyl-ester.pdf>

Generated by Cheméo on 2024-04-28 20:05:27.758026282 +0000 UTC m=+16623976.678603604.

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