

P-anisic acid, 2-adamantyl ester

Inchi: InChI=1S/C18H22O3/c1-20-16-4-2-13(3-5-16)18(19)21-17-14-7-11-6-12(9-14)10-15(17)8
InchiKey: MYDJZALKVKBFFE-UHFFFAOYSA-N
Formula: C18H22O3
SMILES: COc1ccc(C(=O)OC2C3CC4CC(C3)CC2C4)cc1
Mol. weight [g/mol]: 286.37

Physical Properties

Property code	Value	Unit	Source
hf	-536.13	kJ/mol	Cheméo Relay (1.0)
hfus	34.45	kJ/mol	Joback Method
hvap	100.13	kJ/mol	Cheméo Relay (1.0)
ie	8.35	eV	Cheméo Relay (1.0)
log10ws	-5.46		Cheméo Relay (1.0)
logp	3.677		Crippen Method
mcvol	221.450	ml/mol	McGowan Method
rinpol	2354.70		NIST Webbook
rinpol	2354.70		NIST Webbook
tb	658.37	K	Cheméo Relay (1.0)
tf	463.00	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	703.35	J/mol×K	756.76	Joback Method
cpg	723.04	J/mol×K	795.19	Joback Method
cpg	741.32	J/mol×K	833.63	Joback Method
cpg	758.30	J/mol×K	872.06	Joback Method
cpg	774.07	J/mol×K	910.49	Joback Method
cpg	788.75	J/mol×K	948.92	Joback Method
cpg	802.43	J/mol×K	987.36	Joback Method
dvisc	0.0032839	Pa×s	467.77	Joback Method
dvisc	0.0028853	Pa×s	515.93	Joback Method
dvisc	0.0025918	Pa×s	564.10	Joback Method
dvisc	0.0023677	Pa×s	612.27	Joback Method

dvisc	0.0021918	Pa×s	660.43	Joback Method
dvisc	0.0020503	Pa×s	708.60	Joback Method
dvisc	0.0019343	Pa×s	756.76	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U292458&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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