

p-anisic acid, cyclobutyl ester

Inchi:	InChI=1S/C12H14O3/c1-14-10-7-5-9(6-8-10)12(13)15-11-3-2-4-11/h5-8,11H,2-4H2,1H3
InchiKey:	ZGKSQEWTOCGXMB-UHFFFAOYSA-N
Formula:	C12H14O3
SMILES:	COc1ccc(C(=O)OC2CCC2)cc1
Mol. weight [g/mol]:	206.24

Physical Properties

Property code	Value	Unit	Source
hf	-431.19	kJ/mol	Cheméo Relay (1.0)
hfus	20.50	kJ/mol	Joback Method
hvap	81.48	kJ/mol	Cheméo Relay (1.0)
ie	8.48	eV	Cheméo Relay (1.0)
log10ws	-3.55		Cheméo Relay (1.0)
logp	2.405		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinpol	1714.80		NIST Webbook
rinpol	1714.80		NIST Webbook
tb	578.94	K	Cheméo Relay (1.0)
tf	289.14	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.05	J/mol×K	615.34	Joback Method
cpg	422.10	J/mol×K	653.11	Joback Method
cpg	437.11	J/mol×K	690.88	Joback Method
cpg	451.11	J/mol×K	728.65	Joback Method
cpg	464.13	J/mol×K	766.42	Joback Method
cpg	476.19	J/mol×K	804.19	Joback Method
cpg	487.32	J/mol×K	841.96	Joback Method
dvisc	0.0014728	Pa×s	372.75	Joback Method
dvisc	0.0009650	Pa×s	413.18	Joback Method
dvisc	0.0006818	Pa×s	453.61	Joback Method
dvisc	0.0005099	Pa×s	494.04	Joback Method

dvisc	0.0003985	Pa×s	534.48	Joback Method
dvisc	0.0003224	Pa×s	574.91	Joback Method
dvisc	0.0002682	Pa×s	615.34	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U292456&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

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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