

Cyclobutanecarboxylic acid, 4-methoxyphenyl ester

Inchi:	InChI=1S/C12H14O3/c1-14-10-5-7-11(8-6-10)15-12(13)9-3-2-4-9/h5-9H,2-4H2,1H3
InchiKey:	DNZCZKNTHJOOQO-UHFFFAOYSA-N
Formula:	C12H14O3
SMILES:	COc1ccc(OC(=O)C2CCC2)cc1
Mol. weight [g/mol]:	206.24

Physical Properties

Property code	Value	Unit	Source
gf	-137.33	kJ/mol	Joback Method
hf	-376.33	kJ/mol	Joback Method
hfus	20.50	kJ/mol	Joback Method
hvap	56.90	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.401		Crippen Method
mvol	158.630	ml/mol	McGowan Method
pc	2859.68	kPa	Joback Method
rinpol	1637.00		NIST Webbook
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tb	615.34	K	Joback Method
tc	841.96	K	Joback Method
tf	372.75	K	Joback Method
vc	0.591	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.05	J/molxK	615.34	Joback Method
cpg	422.10	J/molxK	653.11	Joback Method
cpg	437.11	J/molxK	690.88	Joback Method
cpg	451.11	J/molxK	728.65	Joback Method
cpg	464.13	J/molxK	766.42	Joback Method
cpg	476.19	J/molxK	804.19	Joback Method
cpg	487.32	J/molxK	841.96	Joback Method
dvisc	0.0014728	Paxs	372.75	Joback Method

dvisc	0.0009650	Paxs	413.18	Joback Method
dvisc	0.0006818	Paxs	453.61	Joback Method
dvisc	0.0005099	Paxs	494.04	Joback Method
dvisc	0.0003985	Paxs	534.48	Joback Method
dvisc	0.0003224	Paxs	574.91	Joback Method
dvisc	0.0002682	Paxs	615.34	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=U307439&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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