

Benzene-1,2-dicarboxylic acid, 3-methoxy, dimethyl ester

Inchi:	InChI=1S/C11H12O5/c1-14-8-6-4-5-7(10(12)15-2)9(8)11(13)16-3/h4-6H,1-3H3
InchiKey:	KKSNRHOMXHCRGF-UHFFFAOYSA-N
Formula:	C11H12O5
SMILES:	<chem>COC(=O)c1cccc(OC)c1C(=O)OC</chem>
Mol. weight [g/mol]:	224.21

Physical Properties

Property code	Value	Unit	Source
gf	-437.95	kJ/mol	Joback Method
hf	-678.60	kJ/mol	Joback Method
hfus	24.27	kJ/mol	Joback Method
hvap	64.40	kJ/mol	Joback Method
log10ws	-2.08		Crippen Method
logp	1.268		Crippen Method
mcvol	162.840	ml/mol	McGowan Method
pc	2775.92	kPa	Joback Method
rinqol	1639.00		NIST Webbook
tb	662.72	K	Joback Method
tc	876.45	K	Joback Method
tf	431.74	K	Joback Method
vc	0.610	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	410.14	J/molxK	662.72	Joback Method
cpg	464.41	J/molxK	840.83	Joback Method
cpg	455.09	J/molxK	805.21	Joback Method
cpg	444.98	J/molxK	769.58	Joback Method
cpg	434.10	J/molxK	733.96	Joback Method
cpg	422.48	J/molxK	698.34	Joback Method
cpg	472.91	J/molxK	876.45	Joback Method
dvisc	0.0001295	Paxs	662.72	Joback Method
dvisc	0.0001580	Paxs	624.22	Joback Method

dvisc	0.0001978	Paxs	585.73	Joback Method
dvisc	0.0002557	Paxs	547.23	Joback Method
dvisc	0.0003435	Paxs	508.73	Joback Method
dvisc	0.0004844	Paxs	470.24	Joback Method
dvisc	0.0007263	Paxs	431.74	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=R306844&Units=SI
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
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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