

endo-Methylenetetrahydrophthalic acid, dimethyl ester

Inchi:	InChI=1S/C11H14O4/c1-14-10(12)8-6-3-4-7(5-6)9(8)11(13)15-2/h3-4,6-9H,5H2,1-2H3
InchiKey:	VGQLNJWOULYV-FV-UHFFFAOYSA-N
Formula:	C11H14O4
SMILES:	COC(=O)C1C2C=CC(C2)C1C(=O)OC
Mol. weight [g/mol]:	210.23

Physical Properties

Property code	Value	Unit	Source
gf	-302.16	kJ/mol	Joback Method
hf	-603.43	kJ/mol	Joback Method
hfus	27.35	kJ/mol	Joback Method
hvap	58.06	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	0.771		Crippen Method
mvol	154.710	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1441.60		NIST Webbook
rinpol	1441.60		NIST Webbook
tb	611.23	K	Joback Method
tc	821.35	K	Joback Method
tf	382.69	K	Joback Method
vc	0.590	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	420.20	J/molxK	611.23	Joback Method
cpg	435.68	J/molxK	646.25	Joback Method
cpg	450.23	J/molxK	681.27	Joback Method
cpg	463.89	J/molxK	716.29	Joback Method
cpg	476.69	J/molxK	751.31	Joback Method
cpg	488.65	J/molxK	786.33	Joback Method
cpg	499.80	J/molxK	821.35	Joback Method
dvisc	0.0020246	Paxs	382.69	Joback Method

dvisc	0.0017265	Paxs	420.78	Joback Method
dvisc	0.0015118	Paxs	458.87	Joback Method
dvisc	0.0013510	Paxs	496.96	Joback Method
dvisc	0.0012267	Paxs	535.05	Joback Method
dvisc	0.0011283	Paxs	573.14	Joback Method
dvisc	0.0010487	Paxs	611.23	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U352615&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

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