Dimethyl 1,4-cyclohexadiene-1,2-dicarboxylate

Inchi: InChI=1S/C10H12O4/c1-13-9(11)7-5-3-4-6-8(7)10(12)14-2/h3-4H,5-6H2,1-2H3
InchiKey: LHDSILFDQOEEGI-UHFFFAOYSA-N
Formula: C10H12O4
SMILES: COC(=O)C1=C(C(=O)OC)CC=CC1
Mol. weight [g/mol]: 196.20
CAS: 14309-54-7

Physical Properties

Property code	Value	Unit	Source
gf	-361.70	kJ/mol	Joback Method
hf	-572.05	kJ/mol	Joback Method
hfus	19.66	kJ/mol	Joback Method
hvap	58.81	kJ/mol	Joback Method
log10ws	-1.34		Crippen Method
logp	0.979		Crippen Method
mcvol	147.180	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
tb	613.28	K	Joback Method
tc	830.36	K	Joback Method
tf	384.96	K	Joback Method
vc	0.549	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	359.89	J/mol×K	613.28	Joback Method
cpg	372.95	J/mol×K	649.46	Joback Method
cpg	385.26	J/mol×K	685.64	Joback Method
cpg	396.82	J/mol×K	721.82	Joback Method
cpg	407.63	J/mol×K	758.00	Joback Method
cpg	417.68	J/mol×K	794.18	Joback Method
cpg	426.96	J/mol×K	830.36	Joback Method
dvisc	0.0013061	Pa×s	384.96	Joback Method
dvisc	0.0008058	Pa×s	423.01	Joback Method

dvisc	0.0005385	Pa×s	461.07	Joback Method
dvisc	0.0003826	Pa×s	499.12	Joback Method
dvisc	0.0002853	Pa×s	537.17	Joback Method
dvisc	0.0002212	Pa×s	575.23	Joback Method
dvisc	0.0001770	Pa×s	613.28	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=C14309547&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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