

Cyclopentylsuccinic acid, methyl ester

Inchi:	InChI=1S/C11H18O4/c1-14-10(12)7-9(11(13)15-2)8-5-3-4-6-8/h8-9H,3-7H2,1-2H3
InchiKey:	XTKLJYGBEOUDEA-UHFFFAOYSA-N
Formula:	C11H18O4
SMILES:	<chem>COC(=O)CC(C(=O)OC)C1CCCC1</chem>
Mol. weight [g/mol]:	214.26

Physical Properties

Property code	Value	Unit	Source
gf	-391.99	kJ/mol	Joback Method
hf	-704.77	kJ/mol	Joback Method
hfus	20.23	kJ/mol	Joback Method
hvap	58.26	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.529		Crippen Method
mcvol	169.870	ml/mol	McGowan Method
pc	2515.07	kPa	Joback Method
rinpol	1490.00		NIST Webbook
tb	618.50	K	Joback Method
tc	823.95	K	Joback Method
tf	353.95	K	Joback Method
vc	0.634	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.24	J/mol×K	618.50	Joback Method
cpg	470.50	J/mol×K	652.74	Joback Method
cpg	485.86	J/mol×K	686.98	Joback Method
cpg	500.33	J/mol×K	721.22	Joback Method
cpg	513.90	J/mol×K	755.47	Joback Method
cpg	526.60	J/mol×K	789.71	Joback Method
cpg	538.42	J/mol×K	823.95	Joback Method
dvisc	0.0025842	Paxs	353.95	Joback Method
dvisc	0.0013684	Paxs	398.04	Joback Method

dvisc	0.0008226	Paxs	442.13	Joback Method
dvisc	0.0005423	Paxs	486.23	Joback Method
dvisc	0.0003831	Paxs	530.32	Joback Method
dvisc	0.0002855	Paxs	574.41	Joback Method
dvisc	0.0002219	Paxs	618.50	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=R292567&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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