

1,4-Cyclohexadiene-1-carboxylic acid, methyl ester

Other names:	Methyl 2,5-dihydrobenzoate
Inchi:	InChI=1S/C8H10O2/c1-10-8(9)7-5-3-2-4-6-7/h2-3,6H,4-5H2,1H3
InchiKey:	MQVGWLAOVAXSOP-UHFFFAOYSA-N
Formula:	C8H10O2
SMILES:	COC(=O)C1=CCC=CC1
Mol. weight [g/mol]:	138.16
CAS:	50983-21-6

Physical Properties

Property code	Value	Unit	Source
gf	-134.99	kJ/mol	Joback Method
hf	-274.50	kJ/mol	Joback Method
hfus	12.08	kJ/mol	Joback Method
hvap	44.54	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.436		Crippen Method
mcvol	111.560	ml/mol	McGowan Method
pc	3695.46	kPa	Joback Method
rinpol	1324.00		NIST Webbook
rinpol	1324.00		NIST Webbook
tb	486.25	K	Joback Method
tc	703.70	K	Joback Method
tf	277.74	K	Joback Method
vc	0.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.49	J/mol×K	486.25	Joback Method
cpg	243.28	J/mol×K	522.49	Joback Method
cpg	255.39	J/mol×K	558.73	Joback Method
cpg	266.82	J/mol×K	594.97	Joback Method
cpg	277.59	J/mol×K	631.21	Joback Method
cpg	287.71	J/mol×K	667.46	Joback Method

cpg	297.20	J/mol×K	703.70	Joback Method
dvisc	0.0027462	Pa×s	277.74	Joback Method
dvisc	0.0014698	Pa×s	312.49	Joback Method
dvisc	0.0008915	Pa×s	347.24	Joback Method
dvisc	0.0005922	Pa×s	382.00	Joback Method
dvisc	0.0004212	Pa×s	416.75	Joback Method
dvisc	0.0003157	Pa×s	451.50	Joback Method
dvisc	0.0002466	Pa×s	486.25	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C50983216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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

Latest version available from:

<https://www.chemeo.com/cid/81-358-5/1-4-Cyclohexadiene-1-carboxylic-acid-methyl-ester.pdf>

Generated by Cheméo on 2025-12-05 20:28:50.257914012 +0000 UTC m=+4714727.787954673.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.