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]: 138.17

Physical Properties

Property code	Value	Unit	Source
hf	-196.29	kJ/mol	Cheméo Relay (1.0)
hfus	12.08	kJ/mol	Joback Method
ie	9.19	eV	Cheméo Relay (1.0)
log10ws	-1.68		Cheméo Relay (1.0)
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	464.16	K	Cheméo Relay (1.0)
tf	260.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.49	J/mol×K	486.25	Joback Method
cpg	297.20	J/mol×K	703.70	Joback Method
cpg	287.71	J/mol×K	667.46	Joback Method
cpg	277.59	J/mol×K	631.21	Joback Method
cpg	266.82	J/mol×K	594.97	Joback Method
cpg	255.39	J/mol×K	558.73	Joback Method
cpg	243.28	J/mol×K	522.49	Joback Method
dvisc	0.0005922	Pa×s	382.00	Joback Method
dvisc	0.0002466	Pa×s	486.25	Joback Method
dvisc	0.0003157	Pa×s	451.50	Joback Method

dvisc	0.0004212	Pa×s	416.75	Joback Method
dvisc	0.0027462	Pa×s	277.74	Joback Method
dvisc	0.0008915	Pa×s	347.24	Joback Method
dvisc	0.0014698	Pa×s	312.49	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C50983216&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
hf: Enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
ie: Ionization energy
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
tf: Normal melting (fusion) point