Cyclohexanecarboxylic acid, 3-methylphenyl ester

Other names: 3-methylphenyl cyclohexanecarboxylate
Inchi: InChI=1S/C14H18O2/c1-11-6-5-9-13(10-11)16-14(15)12-7-3-2-4-8-12/h5-6,9-10,12H,2-4
InchiKey: WSOGYYKXYMIDJU-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: Cc1cccc(OC(=O)C2CCCCC2)c1
Mol. weight [g/mol]: 218.29
CAS: 18731-59-4

Physical Properties

Property code	Value	Unit	Source
gf	-39.69	kJ/mol	Joback Method
hf	-297.71	kJ/mol	Joback Method
hfus	20.29	kJ/mol	Joback Method
hvap	59.28	kJ/mol	Joback Method
log10ws	-4.01		Crippen Method
logp	3.481		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2512.55	kPa	Joback Method
rinpol	1697.00		NIST Webbook
rinpol	1697.00		NIST Webbook
tb	647.22	K	Joback Method
tc	883.33	K	Joback Method
tf	366.02	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.45	J/mol×K	647.22	Joback Method
cpg	504.77	J/mol×K	686.57	Joback Method
cpg	522.71	J/mol×K	725.92	Joback Method
cpg	539.31	J/mol×K	765.27	Joback Method
cpg	554.61	J/mol×K	804.63	Joback Method
cpg	568.65	J/mol×K	843.98	Joback Method

cpg	581.47	J/mol×K	883.33	Joback Method
dvisc	0.0019353	Pa×s	366.02	Joback Method
dvisc	0.0010080	Pa×s	412.89	Joback Method
dvisc	0.0005997	Pa×s	459.75	Joback Method
dvisc	0.0003927	Pa×s	506.62	Joback Method
dvisc	0.0002763	Pa×s	553.49	Joback Method
dvisc	0.0002054	Pa×s	600.35	Joback Method
dvisc	0.0001594	Pa×s	647.22	Joback Method

Sources

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=C18731594&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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