2,2-Dimethylpropionic acid, cyclohexyl ester

Other names: 2,2-Dimethylpropionic acid, cyclohexyl ester
Cyclohexyl pivalate
Inchi: InChI=1S/C11H20O2/c1-11(2,3)10(12)13-9-7-5-4-6-8-9/h9H,4-8H2,1-3H3
InchiKey: WDCXGSMKFYMFCM-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CC(C)(C)C(=O)OC1CCCCC1
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
hf	-563.66	kJ/mol	Cheméo Relay (1.0)
hfus	11.45	kJ/mol	Joback Method
hvap	59.00	kJ/mol	NIST Webbook
log10ws	-3.05		Cheméo Relay (1.0)
logp	2.908		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
tb	485.32	K	Cheméo Relay (1.0)
tf	241.43	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.96	J/mol×K	543.69	Joback Method
cpg	426.73	J/mol×K	579.52	Joback Method
cpg	445.33	J/mol×K	615.35	Joback Method
cpg	462.79	J/mol×K	651.18	Joback Method
cpg	479.14	J/mol×K	687.01	Joback Method
cpg	494.43	J/mol×K	722.84	Joback Method
cpg	508.69	J/mol×K	758.67	Joback Method
dvisc	0.0050998	Pa×s	295.69	Joback Method
dvisc	0.0021528	Pa×s	337.02	Joback Method
dvisc	0.0010972	Pa×s	378.36	Joback Method
dvisc	0.0006386	Pa×s	419.69	Joback Method
dvisc	0.0004096	Pa×s	461.02	Joback Method

dvisc	0.0002826	Pa×s	502.36	Joback Method
dvisc	0.0002063	Pa×s	543.69	Joback Method

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C29878497&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

Legend

cpg: Ideal gas heat capacity
dvisc: Dynamic viscosity
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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point