Cyclohexanecarboxylic acid isopropyl ester

Other names:	Cyclohexanecarboxylic acid, 1-methylethyl ester
	isopropyl cyclohexanecarboxylate
Inchi:	InChI=1S/C10H18O2/c1-8(2)12-10(11)9-6-4-3-5-7-9/h8-9H,3-7H2,1-2H3
InchiKey:	PMQZNGSMBAGPRU-UHFFFAOYSA-N
Formula:	C10H18O2
SMILES:	CC(C)OC(=O)C1CCCCC1
Mol. weight [g/mol]:	170.25
CAS:	6553-80-6

Physical Properties

Property code	Value	Unit	Source
gf	-178.59	kJ/mol	Joback Method
hf	-445.49	kJ/mol	Joback Method
hfus	12.75	kJ/mol	Joback Method
hvap	47.05	kJ/mol	Joback Method
log10ws	-2.64		Crippen Method
logp	2.518		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
tb	523.60	K	Joback Method
tc	733.51	K	Joback Method
tf	267.00	K	Joback Method
vc	0.546	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.54	J/mol×K	523.60	Joback Method
cpg	437.82	J/mol×K	698.52	Joback Method
cpg	423.20	J/mol×K	663.54	Joback Method
cpg	407.67	J/mol×K	628.55	Joback Method
cpg	391.23	J/mol×K	593.57	Joback Method
cpg	373.86	J/mol×K	558.58	Joback Method
cpg	451.55	J/mol×K	733.51	Joback Method

dvisc	0.0002279	Pa×s	523.60	Joback Method
dvisc	0.0003085	Pa×s	480.83	Joback Method
dvisc	0.0004430	Pa×s	438.07	Joback Method
dvisc	0.0006880	Pa×s	395.30	Joback Method
dvisc	0.0011889	Pa×s	352.53	Joback Method
dvisc	0.0023895	Pa×s	309.77	Joback Method
dvisc	0.0060058	Pa×s	267.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6553806&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume