Propanoic acid, 2-methyl-, cyclohexyl ester

Other names: Cyclohexyl iso-butyrate
Inchi: InChI=1S/C10H18O2/c1-8(2)10(11)12-9-6-4-3-5-7-9/h8-9H,3-7H2,1-2H3
InchiKey: IYYXBWAISHVFEX-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CC(C)C(=O)OC1CCCCC1
Mol. weight [g/mol]: 170.25
CAS: 1129-47-1

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	57.70	kJ/mol	NIST Webbook
log10ws	-2.64		Crippen Method
logp	2.518		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2715.50	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
ripol	1427.00		NIST Webbook
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	373.86	J/mol×K	558.58	Joback Method
cpg	391.23	J/mol×K	593.57	Joback Method
cpg	407.67	J/mol×K	628.55	Joback Method
cpg	423.20	J/mol×K	663.54	Joback Method

cpg	437.82	J/mol×K	698.52	Joback Method
cpg	451.55	J/mol×K	733.51	Joback Method
dvisc	0.0060058	Pa×s	267.00	Joback Method
dvisc	0.0023895	Pa×s	309.77	Joback Method
dvisc	0.0011889	Pa×s	352.53	Joback Method
dvisc	0.0006880	Pa×s	395.30	Joback Method
dvisc	0.0004430	Pa×s	438.07	Joback Method
dvisc	0.0003085	Pa×s	480.83	Joback Method
dvisc	0.0002279	Pa×s	523.60	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1129471&Units=SI

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

Latest version available from: