Cyclohexyl isovalerate

Other names: Isovaleric acid cyclohexyl ester
Butanoic acid, 3-methyl-, cyclohexyl ester
Inchi: InChI=1S/C11H20O2/c1-9(2)8-11(12)13-10-6-4-3-5-7-10/h9-10H,3-8H2,1-2H3
InchiKey: SQPOKBBCNZIWFI-UHFFFAOYSA-N
Formula: C11H20O2
SMILES: CC(C)CC(=O)OC1CCCCC1
Mol. weight [g/mol]: 184.28
CAS: 7774-44-9

Physical Properties

Property code	Value	Unit	Source
gf	-170.17	kJ/mol	Joback Method
hf	-466.13	kJ/mol	Joback Method
hfus	15.34	kJ/mol	Joback Method
hvap	49.28	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.908		Crippen Method
mcvol	162.430	ml/mol	McGowan Method
pc	2462.92	kPa	Joback Method
rinpol	1264.00		NIST Webbook
ripol	1527.00		NIST Webbook
tb	546.48	K	Joback Method
tc	753.14	K	Joback Method
tf	278.27	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.33	J/mol×K	546.48	Joback Method
cpg	489.53	J/mol×K	718.70	Joback Method
cpg	474.40	J/mol×K	684.25	Joback Method
cpg	458.33	J/mol×K	649.81	Joback Method
cpg	441.31	J/mol×K	615.37	Joback Method

cpg	423.31	J/mol×K	580.92	Joback Method
cpg	503.73	J/mol×K	753.14	Joback Method
dvisc	0.0002083	Pa×s	546.48	Joback Method
dvisc	0.0002828	Pa×s	501.78	Joback Method
dvisc	0.0004077	Pa×s	457.08	Joback Method
dvisc	0.0006363	Pa×s	412.38	Joback Method
dvisc	0.0011064	Pa×s	367.67	Joback Method
dvisc	0.0022424	Pa×s	322.97	Joback Method
dvisc	0.0057025	Pa×s	278.27	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=C7774449&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

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