Cyclohexanecarboxylic acid, propyl ester

Other names: propyl cyclohexanecarboxylate
Inchi: InChI=1S/C10H18O2/c1-2-8-12-10(11)9-6-4-3-5-7-9/h9H,2-8H2,1H3
InchiKey: UBEVLTHYAFYOEU-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCCOC(=O)C1CCCCC1
Mol. weight [g/mol]: 170.25
CAS: 6739-34-0

Physical Properties

Property code	Value	Unit	Source
gf	-176.15	kJ/mol	Joback Method
hf	-440.21	kJ/mol	Joback Method
hfus	16.28	kJ/mol	Joback Method
hvap	47.44	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.520		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2693.00	kPa	Joback Method
rinpol	1209.00		NIST Webbook
rinpol	1205.98		NIST Webbook
tb	524.04	K	Joback Method
tc	729.39	K	Joback Method
tf	282.00	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	355.31	J/mol×K	524.04	Joback Method
cpg	435.73	J/mol×K	695.17	Joback Method
cpg	421.39	J/mol×K	660.94	Joback Method
cpg	406.18	J/mol×K	626.72	Joback Method
cpg	390.11	J/mol×K	592.49	Joback Method
cpg	373.16	J/mol×K	558.27	Joback Method

cpg	449.24	J/mol×K	729.39	Joback Method
dvisc	0.0002418	Pa×s	524.04	Joback Method
dvisc	0.0003191	Pa×s	483.70	Joback Method
dvisc	0.0004431	Pa×s	443.36	Joback Method
dvisc	0.0006569	Pa×s	403.02	Joback Method
dvisc	0.0010632	Pa×s	362.68	Joback Method
dvisc	0.0019412	Pa×s	322.34	Joback Method
dvisc	0.0042103	Pa×s	282.00	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6739340&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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

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

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