Cyclohexanecarboxylic acid, pentyl ester

Other names: pentyl cyclohexanecarboxylate
Inchi: InChI=1S/C12H22O2/c1-2-3-7-10-14-12(13)11-8-5-4-6-9-11/h11H,2-10H2,1H3
InchiKey: QLFARUWYJWNPLX-UHFFFAOYSA-N
Formula: C12H22O2
SMILES: CCCCCOC(=O)C1CCCCC1
Mol. weight [g/mol]: 198.30
CAS: 6553-83-9

Physical Properties

Property code	Value	Unit	Source
gf	-159.31	kJ/mol	Joback Method
hf	-481.49	kJ/mol	Joback Method
hfus	21.46	kJ/mol	Joback Method
hvap	51.89	kJ/mol	Joback Method
log10ws	-3.36		Crippen Method
logp	3.300		Crippen Method
mcvol	176.520	ml/mol	McGowan Method
pc	2227.09	kPa	Joback Method
rinpol	1405.39		NIST Webbook
rinpol	1408.57		NIST Webbook
tb	569.80	K	Joback Method
tc	769.23	K	Joback Method
tf	304.54	K	Joback Method
vc	0.664	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	454.49	J/mol×K	569.80	Joback Method
cpg	540.32	J/mol×K	735.99	Joback Method
cpg	525.03	J/mol×K	702.75	Joback Method
cpg	508.82	J/mol×K	669.52	Joback Method
cpg	491.68	J/mol×K	636.28	Joback Method
cpg	473.57	J/mol×K	603.04	Joback Method

cpg	554.70	J/mol×K	769.23	Joback Method
dvisc	0.0002015	Pa×s	569.80	Joback Method
dvisc	0.0002680	Pa×s	525.59	Joback Method
dvisc	0.0003757	Pa×s	481.38	Joback Method
dvisc	0.0005638	Pa×s	437.17	Joback Method
dvisc	0.0009272	Pa×s	392.96	Joback Method
dvisc	0.0017297	Pa×s	348.75	Joback Method
dvisc	0.0038673	Pa×s	304.54	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=C6553839&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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