3-Cyclopentylpropionic acid, ethyl ester

Inchi: InChI=1S/C10H18O2/c1-2-12-10(11)8-7-9-5-3-4-6-9/h9H,2-8H2,1H3
InchiKey: XBPSVBXDXASTJT-UHFFFAOYSA-N
Formula: C10H18O2
SMILES: CCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 170.25
CAS: 17931-64-5

Physical Properties

Property code	Value	Unit	Source
gf	-164.05	kJ/mol	Joback Method
hf	-434.05	kJ/mol	Joback Method
hfus	18.38	kJ/mol	Joback Method
hvap	47.27	kJ/mol	Joback Method
log10ws	-2.52		Crippen Method
logp	2.520		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	2624.46	kPa	Joback Method
rinpol	1250.00		NIST Webbook
rinpol	1250.00		NIST Webbook
tb	519.77	K	Joback Method
tc	717.95	K	Joback Method
tf	285.52	K	Joback Method
vc	0.560	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	354.79	J/mol×K	519.77	Joback Method
cpg	371.67	J/mol×K	552.80	Joback Method
cpg	387.71	J/mol×K	585.83	Joback Method
cpg	402.95	J/mol×K	618.86	Joback Method
cpg	417.39	J/mol×K	651.89	Joback Method
cpg	431.06	J/mol×K	684.92	Joback Method
cpg	443.98	J/mol×K	717.95	Joback Method

dvisc	0.0033634	Pa×s	285.52	Joback Method
dvisc	0.0017645	Pa×s	324.56	Joback Method
dvisc	0.0010632	Pa×s	363.60	Joback Method
dvisc	0.0007068	Pa×s	402.64	Joback Method
dvisc	0.0005050	Pa×s	441.69	Joback Method
dvisc	0.0003811	Pa×s	480.73	Joback Method
dvisc	0.0003000	Pa×s	519.77	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=C17931645&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