3-Cyclopentylpropionic acid, 4-methoxy-2-methylbutyl ester

Inchi: InChI=1S/C14H26O3/c1-12(9-10-16-2)11-17-14(15)8-7-13-5-3-4-6-13/h12-13H,3-11H2,1

InchiKey: QBAANVKOMZFPGW-UHFFFAOYSA-N

Formula: C14H26O3

SMILES: COCCC(C)COC(=O)CCC1CCCC1

Mol. weight [g/mol]: 242.35

Physical Properties

Property code	Value	Unit	Source
gf	-237.81	kJ/mol	Joback Method
hf	-654.11	kJ/mol	Joback Method
hfus	26.40	kJ/mol	Joback Method
hvap	58.19	kJ/mol	Joback Method
log10ws	-3.04		Crippen Method
logp	3.173		Crippen Method
mcvol	210.570	ml/mol	McGowan Method
pc	1818.50	kPa	Joback Method
rinpol	1755.00		NIST Webbook
tb	633.27	K	Joback Method
tc	823.95	K	Joback Method
tf	337.83	K	Joback Method
vc	0.796	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	587.91	J/mol×K	633.27	Joback Method
cpg	673.43	J/mol×K	792.17	Joback Method
cpg	658.19	J/mol×K	760.39	Joback Method
cpg	642.04	J/mol×K	728.61	Joback Method
cpg	624.95	J/mol×K	696.83	Joback Method
cpg	606.91	J/mol×K	665.05	Joback Method
cpg	687.76	J/mol×K	823.95	Joback Method
dvisc	0.0001576	Pa×s	633.27	Joback Method
dvisc	0.0002076	Pa×s	584.03	Joback Method

dvisc	0.0002876	Pa×s	534.79	Joback Method
dvisc	0.0004256	Pa×s	485.55	Joback Method
dvisc	0.0006883	Pa×s	436.31	Joback Method
dvisc	0.0012577	Pa×s	387.07	Joback Method
dvisc	0.0027399	Pa×s	337.83	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354332&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

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