3-Cyclopentylpropionic acid, 3-methylbutyl ester

Inchi: InChI=1S/C13H24O2/c1-11(2)9-10-15-13(14)8-7-12-5-3-4-6-12/h11-12H,3-10H2,1-2H3
InchiKey: VXUPUVJRNMABKJ-UHFFFAOYSA-N
Formula: C13H24O2
SMILES: CC(C)CCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 212.33

Physical Properties

Property code	Value	Unit	Source
gf	-141.23	kJ/mol	Joback Method
hf	-501.25	kJ/mol	Joback Method
hfus	22.62	kJ/mol	Joback Method
hvap	53.56	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.546		Crippen Method
mcvol	190.610	ml/mol	McGowan Method
pc	2007.30	kPa	Joback Method
rinpol	1535.00		NIST Webbook
rinpol	1535.00		NIST Webbook
tb	587.97	K	Joback Method
tc	782.26	K	Joback Method
tf	304.33	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.00	J/mol×K	587.97	Joback Method
cpg	524.05	J/mol×K	620.35	Joback Method
cpg	542.13	J/mol×K	652.73	Joback Method
cpg	559.26	J/mol×K	685.12	Joback Method
cpg	575.47	J/mol×K	717.50	Joback Method
cpg	590.78	J/mol×K	749.88	Joback Method
cpg	605.21	J/mol×K	782.26	Joback Method
dvisc	0.0041530	Pa×s	304.33	Joback Method

dvisc	0.0018328	Pa×s	351.60	Joback Method
dvisc	0.0009819	Pa×s	398.88	Joback Method
dvisc	0.0006004	Pa×s	446.15	Joback Method
dvisc	0.0004035	Pa×s	493.42	Joback Method
dvisc	0.0002906	Pa×s	540.70	Joback Method
dvisc	0.0002207	Pa×s	587.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354328&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