3-Cyclopentylpropionic acid, tridecyl ester

Inchi: InChI=1S/C21H40O2/c1-2-3-4-5-6-7-8-9-10-11-14-19-23-21(22)18-17-20-15-12-13-16-20
InchiKey: GQDYEEAXSXIUTM-UHFFFAOYSA-N
Formula: C21H40O2
SMILES: CCCCCCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 324.54

Physical Properties

Property code	Value	Unit	Source
gf	-71.43	kJ/mol	Joback Method
hf	-661.09	kJ/mol	Joback Method
hfus	46.87	kJ/mol	Joback Method
hvap	71.75	kJ/mol	Joback Method
log10ws	-7.13		Crippen Method
logp	6.811		Crippen Method
mcvol	303.330	ml/mol	McGowan Method
pc	1105.21	kPa	Joback Method
rinpol	2351.10		NIST Webbook
rinpol	2351.10		NIST Webbook
tb	771.45	K	Joback Method
tc	955.43	K	Joback Method
tf	409.49	K	Joback Method
vc	1.177	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	963.47	J/mol×K	771.45	Joback Method
cpg	984.35	J/mol×K	802.11	Joback Method
cpg	1004.10	J/mol×K	832.78	Joback Method
cpg	1022.76	J/mol×K	863.44	Joback Method
cpg	1040.36	J/mol×K	894.10	Joback Method
cpg	1056.95	J/mol×K	924.77	Joback Method
cpg	1072.55	J/mol×K	955.43	Joback Method
dvisc	0.0017770	Pa×s	409.49	Joback Method

dvisc	0.0007945	Pa×s	469.82	Joback Method
dvisc	0.0004267	Pa×s	530.14	Joback Method
dvisc	0.0002602	Pa×s	590.47	Joback Method
dvisc	0.0001739	Pa×s	650.80	Joback Method
dvisc	0.0001244	Pa×s	711.12	Joback Method
dvisc	0.0000938	Pa×s	771.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U292337&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