3-Cyclopentylpropionic acid, heptadecyl ester

Inchi: InChI=1S/C25H48O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-23-27-25(26)22-21-24-19
InchiKey: WJHIYBFCQQGWNY-UHFFFAOYSA-N
Formula: C25H48O2
SMILES: CCCCCCCCCCCCCCCCCCOC(=O)CCC1CCCC1
Mol. weight [g/mol]: 380.65

Physical Properties

Property code	Value	Unit	Source
gf	-37.75	kJ/mol	Joback Method
hf	-743.65	kJ/mol	Joback Method
hfus	57.23	kJ/mol	Joback Method
hvap	80.66	kJ/mol	Joback Method
log10ws	-8.80		Crippen Method
logp	8.371		Crippen Method
mcvol	359.690	ml/mol	McGowan Method
pc	869.14	kPa	Joback Method
rinpol	2701.20		NIST Webbook
tb	862.97	K	Joback Method
tc	1057.10	K	Joback Method
tf	454.57	K	Joback Method
vc	1.401	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1215.31	J/mol×K	862.97	Joback Method
cpg	1237.36	J/mol×K	895.32	Joback Method
cpg	1258.09	J/mol×K	927.68	Joback Method
cpg	1277.55	J/mol×K	960.03	Joback Method
cpg	1295.80	J/mol×K	992.39	Joback Method
cpg	1312.88	J/mol×K	1024.74	Joback Method
cpg	1328.87	J/mol×K	1057.10	Joback Method
dvisc	0.0011563	Pa×s	454.57	Joback Method
dvisc	0.0004975	Pa×s	522.64	Joback Method

dvisc	0.0002600	Pa×s	590.70	Joback Method
dvisc	0.0001554	Pa×s	658.77	Joback Method
dvisc	0.0001022	Pa×s	726.84	Joback Method
dvisc	0.0000723	Pa×s	794.90	Joback Method
dvisc	0.0000540	Pa×s	862.97	Joback Method

Sources

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=U292274&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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