4-Hexadecyl cyclopentanecarboxylate

Inchi: InChI=1S/C22H42O2/c1-3-5-6-7-8-9-10-11-12-13-19-21(16-4-2)24-22(23)20-17-14-15-18
InchiKey: FBBOXFRALFYLMY-UHFFFAOYSA-N
Formula: C22H42O2
SMILES: CCCCCCCCCCCCC(CCC)OC(=O)C1CCCC1
Mol. weight [g/mol]: 338.57

Physical Properties

Property code	Value	Unit	Source
gf	-65.45	kJ/mol	Joback Method
hf	-687.01	kJ/mol	Joback Method
hfus	45.93	kJ/mol	Joback Method
hvap	73.59	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	7.200		Crippen Method
mcvol	317.420	ml/mol	McGowan Method
pc	1043.27	kPa	Joback Method
rinpol	285.10		NIST Webbook
rinpol	285.10		NIST Webbook
tb	793.89	K	Joback Method
tc	980.66	K	Joback Method
tf	405.76	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1025.80	J/mol×K	793.89	Joback Method
cpg	1047.08	J/mol×K	825.02	Joback Method
cpg	1067.16	J/mol×K	856.15	Joback Method
cpg	1086.10	J/mol×K	887.27	Joback Method
cpg	1103.93	J/mol×K	918.40	Joback Method
cpg	1120.68	J/mol×K	949.53	Joback Method
cpg	1136.41	J/mol×K	980.66	Joback Method
dvisc	0.0019486	Pa×s	405.76	Joback Method

dvisc	0.0007807	Pa×s	470.45	Joback Method
dvisc	0.0003902	Pa×s	535.14	Joback Method
dvisc	0.0002265	Pa×s	599.83	Joback Method
dvisc	0.0001462	Pa×s	664.51	Joback Method
dvisc	0.0001020	Pa×s	729.20	Joback Method
dvisc	0.0000754	Pa×s	793.89	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=R516655&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