Hexadecanoic acid, cyclohexyl ester

Other names: Cyclohexyl palmitate
Inchi: InChI=1S/C22H42O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-20-22(23)24-21-18-15-14-16-19
InchiKey: BMZOQYYROAVSAP-UHFFFAOYSA-N
Formula: C22H42O2
SMILES: CCCCCCCCCCCCCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]: 338.57
CAS: 1673-08-1

Physical Properties

Property code	Value	Unit	Source
gf	-75.11	kJ/mol	Joback Method
hf	-687.89	kJ/mol	Joback Method
hfus	47.36	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-7.90		Crippen Method
logp	7.344		Crippen Method
mcvol	317.420	ml/mol	McGowan Method
pc	1054.83	kPa	Joback Method
rinpol	2466.20		NIST Webbook
rinpol	2420.00		NIST Webbook
tb	798.60	K	Joback Method
tc	986.81	K	Joback Method
tf	417.24	K	Joback Method
vc	1.224	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.92	J/mol×K	798.60	Joback Method
cpg	1125.12	J/mol×K	955.44	Joback Method
cpg	1108.43	J/mol×K	924.08	Joback Method
cpg	1090.61	J/mol×K	892.71	Joback Method
cpg	1071.60	J/mol×K	861.34	Joback Method
cpg	1051.39	J/mol×K	829.97	Joback Method

cpg	1140.70	J/mol×K	986.81	Joback Method
dvisc	0.0000578	Pa×s	798.60	Joback Method
dvisc	0.0000790	Pa×s	735.04	Joback Method
dvisc	0.0001143	Pa×s	671.48	Joback Method
dvisc	0.0001789	Pa×s	607.92	Joback Method
dvisc	0.0003107	Pa×s	544.36	Joback Method
dvisc	0.0006244	Pa×s	480.80	Joback Method
dvisc	0.0015525	Pa×s	417.24	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=C1673081&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

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