

Cyclohexyl undecanoate

Inchi: InChI=1S/C17H32O2/c1-2-3-4-5-6-7-8-12-15-17(18)19-16-13-10-9-11-14-16/h16H,2-15H
InchiKey: AEUTTXKLSKPMHY-UHFFFAOYSA-N
Formula: C17H32O2
SMILES: CCCCCCCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]: 268.43

Physical Properties

Property code	Value	Unit	Source
gf	-117.21	kJ/mol	Joback Method
hf	-584.69	kJ/mol	Joback Method
hfus	34.41	kJ/mol	Joback Method
hvap	63.02	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.393		Crippen Method
mcvol	246.970	ml/mol	McGowan Method
pc	1480.43	kPa	Joback Method
rinpol	1906.00		NIST Webbook
tb	684.20	K	Joback Method
tc	872.77	K	Joback Method
tf	360.89	K	Joback Method
vc	0.945	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.28	J/mol×K	684.20	Joback Method
cpg	748.95	J/mol×K	715.63	Joback Method
cpg	768.52	J/mol×K	747.06	Joback Method
cpg	787.02	J/mol×K	778.49	Joback Method
cpg	804.46	J/mol×K	809.92	Joback Method
cpg	820.87	J/mol×K	841.35	Joback Method
cpg	836.28	J/mol×K	872.77	Joback Method
dvisc	0.0026482	Pa×s	360.89	Joback Method
dvisc	0.0011147	Pa×s	414.77	Joback Method

dvisc	0.0005725	Pa×s	468.66	Joback Method
dvisc	0.0003374	Pa×s	522.54	Joback Method
dvisc	0.0002195	Pa×s	576.43	Joback Method
dvisc	0.0001536	Pa×s	630.31	Joback Method
dvisc	0.0001138	Pa×s	684.20	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R541552&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

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