

Cyclohexyl pentadecanoate

Inchi:	InChI=1S/C21H40O2/c1-2-3-4-5-6-7-8-9-10-11-12-16-19-21(22)23-20-17-14-13-15-18-20
InchiKey:	LDGCLFIGEDVJAN-UHFFFAOYSA-N
Formula:	C21H40O2
SMILES:	CCCCCCCCCCCCCCC(=O)OC1CCCCC1
Mol. weight [g/mol]:	324.54

Physical Properties

Property code	Value	Unit	Source
gf	-83.53	kJ/mol	Joback Method
hf	-667.25	kJ/mol	Joback Method
hfus	44.77	kJ/mol	Joback Method
hvap	71.92	kJ/mol	Joback Method
log10ws	-7.48		Crippen Method
logp	6.954		Crippen Method
mcvol	303.330	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	775.72	K	Joback Method
tc	962.87	K	Joback Method
tf	405.97	K	Joback Method
vc	1.169	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.85	J/molxK	775.72	Joback Method
cpg	989.15	J/molxK	806.91	Joback Method
cpg	1009.24	J/molxK	838.10	Joback Method
cpg	1028.16	J/molxK	869.29	Joback Method
cpg	1045.92	J/molxK	900.49	Joback Method
cpg	1062.58	J/molxK	931.68	Joback Method
cpg	1078.15	J/molxK	962.87	Joback Method
dvisc	0.0017434	Paxs	405.97	Joback Method

dvisc	0.0007070	Paxs	467.59	Joback Method
dvisc	0.0003538	Paxs	529.22	Joback Method
dvisc	0.0002045	Paxs	590.85	Joback Method
dvisc	0.0001311	Paxs	652.47	Joback Method
dvisc	0.0000908	Paxs	714.10	Joback Method
dvisc	0.0000666	Paxs	775.72	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R541532&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

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