Benzoic acid, cyclohexyl ester

Other names: Cyclohexyl benzoate
Hexahydrophenyl benzoate
Inchi: InChI=1S/C13H16O2/c14-13(11-7-3-1-4-8-11)15-12-9-5-2-6-10-12/h1,3-4,7-8,12H,2,5-6,
InchiKey: DQZKGSRJOUYVPL-UHFFFAOYSA-N
Formula: C13H16O2
SMILES: O=C(OC1CCCCC1)c1ccccc1
Mol. weight [g/mol]: 204.26
CAS: 2412-73-9

Physical Properties

Property code	Value	Unit	Source
gf	-38.48	kJ/mol	Joback Method
hf	-265.60	kJ/mol	Joback Method
hfus	18.09	kJ/mol	Joback Method
hvap	56.39	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.176		Crippen Method
mcvol	166.850	ml/mol	McGowan Method
pc	2817.33	kPa	Joback Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
tb	619.36	K	Joback Method
tc	859.53	K	Joback Method
tf	342.23	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.78	J/mol×K	619.36	Joback Method
cpg	452.99	J/mol×K	659.39	Joback Method
cpg	470.80	J/mol×K	699.42	Joback Method
cpg	487.25	J/mol×K	739.44	Joback Method
cpg	502.38	J/mol×K	779.47	Joback Method

cpg	516.23	J/mol×K	819.50	Joback Method
cpg	528.86	J/mol×K	859.53	Joback Method
dvisc	0.0026458	Pa×s	342.23	Joback Method
dvisc	0.0012931	Pa×s	388.42	Joback Method
dvisc	0.0007358	Pa×s	434.61	Joback Method
dvisc	0.0004666	Pa×s	480.80	Joback Method
dvisc	0.0003205	Pa×s	526.98	Joback Method
dvisc	0.0002339	Pa×s	573.17	Joback Method
dvisc	0.0001789	Pa×s	619.36	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=C2412739&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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