Benzoic acid, cyclohexylmethyl ester

Inchi: InChI=1S/C14H18O2/c15-14(13-9-5-2-6-10-13)16-11-12-7-3-1-4-8-12/h2,5-6,9-10,12H,1
InchiKey: CINNWVCWEFZMGR-UHFFFAOYSA-N
Formula: C14H18O2
SMILES: O=C(OCC1CCCCC1)c1ccccc1
Mol. weight [g/mol]: 218.29

Physical Properties

Property code	Value	Unit	Source
gf	-30.06	kJ/mol	Joback Method
hf	-286.24	kJ/mol	Joback Method
hfus	20.68	kJ/mol	Joback Method
hvap	58.62	kJ/mol	Joback Method
log10ws	-3.88		Crippen Method
logp	3.424		Crippen Method
mcvol	180.940	ml/mol	McGowan Method
pc	2550.76	kPa	Joback Method
rinpol	1783.00		NIST Webbook
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tb	642.24	K	Joback Method
tc	877.44	K	Joback Method
tf	353.50	K	Joback Method
vc	0.668	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	485.75	J/mol×K	642.24	Joback Method
cpg	569.80	J/mol×K	838.24	Joback Method
cpg	555.65	J/mol×K	799.04	Joback Method
cpg	540.21	J/mol×K	759.84	Joback Method
cpg	523.44	J/mol×K	720.64	Joback Method
cpg	505.31	J/mol×K	681.44	Joback Method
cpg	582.73	J/mol×K	877.44	Joback Method
dvisc	0.0001611	Pa×s	642.24	Joback Method

dvisc	0.0002115	Pa×s	594.12	Joback Method
dvisc	0.0002911	Pa×s	545.99	Joback Method
dvisc	0.0004263	Pa×s	497.87	Joback Method
dvisc	0.0006773	Pa×s	449.75	Joback Method
dvisc	0.0012026	Pa×s	401.62	Joback Method
dvisc	0.0024963	Pa×s	353.50	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=U357799&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