

Cyclohexanecarboxylic acid, 4-biphenyl ester

Inchi: InChI=1S/C19H20O2/c20-19(17-9-5-2-6-10-17)21-18-13-11-16(12-14-18)15-7-3-1-4-8-15
InchiKey: FNFLCKGXSVZHKK-UHFFFAOYSA-N
Formula: C19H20O2
SMILES: O=C(Oc1ccc(-c2ccccc2)cc1)C1CCCCC1
Mol. weight [g/mol]: 280.36

Physical Properties

Property code	Value	Unit	Source
gf	114.82	kJ/mol	Joback Method
hf	-164.38	kJ/mol	Joback Method
hfus	27.28	kJ/mol	Joback Method
hvap	72.69	kJ/mol	Joback Method
log10ws	-6.13		Crippen Method
logp	4.839		Crippen Method
mcvol	227.630	ml/mol	McGowan Method
pc	2175.46	kPa	Joback Method
rinpol	2526.00		NIST Webbook
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tb	788.30	K	Joback Method
tc	1044.24	K	Joback Method
tf	448.79	K	Joback Method
vc	0.841	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	675.42	J/mol×K	788.30	Joback Method
cpg	752.49	J/mol×K	1001.58	Joback Method
cpg	740.30	J/mol×K	958.93	Joback Method
cpg	726.59	J/mol×K	916.27	Joback Method
cpg	711.26	J/mol×K	873.61	Joback Method
cpg	694.24	J/mol×K	830.96	Joback Method
cpg	763.23	J/mol×K	1044.24	Joback Method
dvisc	0.0000901	Pa×s	788.30	Joback Method

dvisc	0.0001163	Pa×s	731.71	Joback Method
dvisc	0.0001568	Pa×s	675.13	Joback Method
dvisc	0.0002233	Pa×s	618.54	Joback Method
dvisc	0.0003413	Pa×s	561.96	Joback Method
dvisc	0.0005738	Pa×s	505.38	Joback Method
dvisc	0.0010998	Pa×s	448.79	Joback Method

Sources

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=U354655&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
mccvol:	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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