3-Cyclopentylpropionic acid, 4-biphenyl ester

Inchi: InChI=1S/C20H22O2/c21-20(15-10-16-6-4-5-7-16)22-19-13-11-18(12-14-19)17-8-2-1-3-9
InchiKey: GKUMHCCEVFDSME-UHFFFAOYSA-N
Formula: C20H22O2
SMILES: O=C(CCC1CCCC1)Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]: 294.39

Physical Properties

Property code	Value	Unit	Source
gf	135.34	kJ/mol	Joback Method
hf	-178.86	kJ/mol	Joback Method
hfus	31.97	kJ/mol	Joback Method
hvap	74.74	kJ/mol	Joback Method
log10ws	-6.55		Crippen Method
logp	5.229		Crippen Method
mcvol	241.720	ml/mol	McGowan Method
pc	1949.23	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	806.91	K	Joback Method
tc	1050.71	K	Joback Method
tf	463.58	K	Joback Method
vc	0.904	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	728.80	J/mol×K	806.91	Joback Method
cpg	746.97	J/mol×K	847.54	Joback Method
cpg	763.56	J/mol×K	888.18	Joback Method
cpg	778.68	J/mol×K	928.81	Joback Method
cpg	792.41	J/mol×K	969.44	Joback Method
cpg	804.84	J/mol×K	1010.08	Joback Method
cpg	816.07	J/mol×K	1050.71	Joback Method
dvisc	0.0011068	Pa×s	463.58	Joback Method

dvisc	0.0006137	Pa×s	520.80	Joback Method
dvisc	0.0003824	Pa×s	578.02	Joback Method
dvisc	0.0002595	Pa×s	635.25	Joback Method
dvisc	0.0001877	Pa×s	692.47	Joback Method
dvisc	0.0001427	Pa×s	749.69	Joback Method
dvisc	0.0001128	Pa×s	806.91	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354061&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