Cyclopentanecarboxylic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C19H20O3/c20-19(16-8-4-5-9-16)22-18-12-10-17(11-13-18)21-14-15-6-2-1-3-7

InchiKey: BKFLQPZYCSQANV-UHFFFAOYSA-N

Formula: C19H20O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C1CCCC1

Mol. weight [g/mol]: 296.36

Physical Properties

Property code	Value	Unit	Source
gf	21.92	kJ/mol	Joback Method
hf	-290.44	kJ/mol	Joback Method
hfus	30.57	kJ/mol	Joback Method
hvap	74.92	kJ/mol	Joback Method
log10ws	-5.34		Crippen Method
logp	4.361		Crippen Method
mcvol	233.500	ml/mol	McGowan Method
pc	2092.66	kPa	Joback Method
rinpol	2454.00		NIST Webbook
tb	806.45	K	Joback Method
tc	1051.39	K	Joback Method
tf	474.54	K	Joback Method
vc	0.867	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	700.00	J/mol×K	806.45	Joback Method
cpg	717.39	J/mol×K	847.27	Joback Method
cpg	733.18	J/mol×K	888.10	Joback Method
cpg	747.43	J/mol×K	928.92	Joback Method
cpg	760.22	J/mol×K	969.74	Joback Method
cpg	771.60	J/mol×K	1010.57	Joback Method
cpg	781.64	J/mol×K	1051.39	Joback Method
dvisc	0.0008659	Pa×s	474.54	Joback Method
dvisc	0.0004978	Pa×s	529.86	Joback Method

dvisc	0.0003177	Pa×s	585.18	Joback Method
dvisc	0.0002192	Pa×s	640.50	Joback Method
dvisc	0.0001604	Pa×s	695.81	Joback Method
dvisc	0.0001229	Pa×s	751.13	Joback Method
dvisc	0.0000976	Pa×s	806.45	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=U307582&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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