Cyclohexanecarboxylic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C20H22O3/c21-20(17-9-5-2-6-10-17)23-19-13-11-18(12-14-19)22-15-16-7-3-1

InchiKey: WFTHGCZJTHGGCB-UHFFFAOYSA-N

Formula: C20H22O3

SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C1CCCCC1

Mol. weight [g/mol]: 310.39

Physical Properties

Property code	Value	Unit	Source
gf	18.24	kJ/mol	Joback Method
hf	-317.24	kJ/mol	Joback Method
hfus	31.06	kJ/mol	Joback Method
hvap	77.32	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.751		Crippen Method
mcvol	247.590	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	2589.00		NIST Webbook
rinpol	2589.00		NIST Webbook
tb	833.60	K	Joback Method
tc	1080.64	K	Joback Method
tf	482.29	K	Joback Method
vc	0.914	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	760.92	J/mol×K	833.60	Joback Method
cpg	832.72	J/mol×K	1039.47	Joback Method
cpg	821.66	J/mol×K	998.29	Joback Method
cpg	809.01	J/mol×K	957.12	Joback Method
cpg	794.71	J/mol×K	915.95	Joback Method
cpg	778.70	J/mol×K	874.77	Joback Method
cpg	842.25	J/mol×K	1080.64	Joback Method
dvisc	0.0000602	Pa×s	833.60	Joback Method

dvisc	0.0000777	Pa×s	775.05	Joback Method
dvisc	0.0001046	Pa×s	716.50	Joback Method
dvisc	0.0001486	Pa×s	657.94	Joback Method
dvisc	0.0002260	Pa×s	599.39	Joback Method
dvisc	0.0003764	Pa×s	540.84	Joback Method
dvisc	0.0007094	Pa×s	482.29	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=U307710&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
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