

3-Cyclopentylpropionic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C21H24O3/c22-21(15-10-17-6-4-5-7-17)24-20-13-11-19(12-14-20)23-16-18-8-
InchiKey: ONWJVVOOXLVMNID-UHFFFAOYSA-N
Formula: C21H24O3
SMILES: O=C(CCC1CCCC1)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]: 324.41

Physical Properties

Property code	Value	Unit	Source
gf	38.76	kJ/mol	Joback Method
hf	-331.72	kJ/mol	Joback Method
hfus	35.75	kJ/mol	Joback Method
hvap	79.38	kJ/mol	Joback Method
log10ws	-6.18		Crippen Method
logp	5.141		Crippen Method
mvol	261.680	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	2684.00		NIST Webbook
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tb	852.21	K	Joback Method
tc	1089.13	K	Joback Method
tf	497.08	K	Joback Method
vc	0.979	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	815.20	J/mol×K	852.21	Joback Method
cpg	886.50	J/mol×K	1049.64	Joback Method
cpg	875.11	J/mol×K	1010.16	Joback Method
cpg	862.35	J/mol×K	970.67	Joback Method
cpg	848.16	J/mol×K	931.18	Joback Method
cpg	832.47	J/mol×K	891.70	Joback Method
cpg	896.60	J/mol×K	1089.13	Joback Method
dvisc	0.0000757	Paxs	852.21	Joback Method

dvisc	0.0000960	Paxs	793.02	Joback Method
dvisc	0.0001264	Paxs	733.83	Joback Method
dvisc	0.0001746	Paxs	674.64	Joback Method
dvisc	0.0002567	Paxs	615.46	Joback Method
dvisc	0.0004098	Paxs	556.27	Joback Method
dvisc	0.0007312	Paxs	497.08	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=U307138&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

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