

Carbonic acid, neopentyl 4-benzyloxyphenyl ester

Inchi:	InChI=1S/C19H22O4/c1-19(2,3)14-22-18(20)23-17-11-9-16(10-12-17)21-13-15-7-5-4-6-8
InchiKey:	YDKLLHCFNJANBE-UHFFFAOYSA-N
Formula:	C19H22O4
SMILES:	CC(C)(C)COC(=O)Oc1ccc(OCc2ccccc2)cc1
Mol. weight [g/mol]:	314.38

Physical Properties

Property code	Value	Unit	Source
gf	-116.79	kJ/mol	Joback Method
hf	-491.89	kJ/mol	Joback Method
hfus	30.41	kJ/mol	Joback Method
hvap	75.78	kJ/mol	Joback Method
log10ws	-5.51		Crippen Method
logp	4.827		Crippen Method
mcvol	250.230	ml/mol	McGowan Method
pc	1789.39	kPa	Joback Method
rinsol	2404.00		NIST Webbook
tb	810.36	K	Joback Method
tc	1038.29	K	Joback Method
tf	488.29	K	Joback Method
vc	0.932	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	739.12	J/molxK	810.36	Joback Method
cpg	755.02	J/molxK	848.35	Joback Method
cpg	769.57	J/molxK	886.34	Joback Method
cpg	782.81	J/molxK	924.32	Joback Method
cpg	794.78	J/molxK	962.31	Joback Method
cpg	805.53	J/molxK	1000.30	Joback Method
cpg	815.11	J/molxK	1038.29	Joback Method
dvisc	0.0004479	Paxs	488.29	Joback Method
dvisc	0.0002453	Paxs	541.97	Joback Method

dvisc	0.0001498	Paxs	595.65	Joback Method
dvisc	0.0000992	Paxs	649.32	Joback Method
dvisc	0.0000700	Paxs	703.00	Joback Method
dvisc	0.0000519	Paxs	756.68	Joback Method
dvisc	0.0000400	Paxs	810.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U357865&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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