

Cyclobutanecarboxylic acid, 4-benzyloxyphenyl ester

Inchi: InChI=1S/C18H18O3/c19-18(15-7-4-8-15)21-17-11-9-16(10-12-17)20-13-14-5-2-1-3-6-14
InchiKey: MLTQEXIFKGNXBF-UHFFFAOYSA-N
Formula: C18H18O3
SMILES: O=C(Oc1ccc(OCc2ccccc2)cc1)C1CCC1
Mol. weight [g/mol]: 282.33

Physical Properties

Property code	Value	Unit	Source
gf	25.60	kJ/mol	Joback Method
hf	-263.64	kJ/mol	Joback Method
hfus	30.08	kJ/mol	Joback Method
hvap	72.53	kJ/mol	Joback Method
log10ws	-4.92		Crippen Method
logp	3.971		Crippen Method
mcvol	219.410	ml/mol	McGowan Method
pc	2235.52	kPa	Joback Method
rinpol	2335.00		NIST Webbook
rinpol	2335.00		NIST Webbook
tb	779.30	K	Joback Method
tc	1022.07	K	Joback Method
tf	466.79	K	Joback Method
vc	0.819	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.37	J/molxK	779.30	Joback Method
cpg	657.17	J/molxK	819.76	Joback Method
cpg	672.51	J/molxK	860.22	Joback Method
cpg	686.49	J/molxK	900.69	Joback Method
cpg	699.16	J/molxK	941.15	Joback Method
cpg	710.60	J/molxK	981.61	Joback Method
cpg	720.88	J/molxK	1022.07	Joback Method
dvisc	0.0010354	Paxs	466.79	Joback Method

dvisc	0.0006439	Paxs	518.88	Joback Method
dvisc	0.0004367	Paxs	570.96	Joback Method
dvisc	0.0003160	Paxs	623.04	Joback Method
dvisc	0.0002404	Paxs	675.13	Joback Method
dvisc	0.0001902	Paxs	727.21	Joback Method
dvisc	0.0001552	Paxs	779.30	Joback Method

Sources

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=U307444&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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