

trans-1,4-dibenzylcyclohexane

Inchi:	InChI=1S/C20H24/c1-3-7-17(8-4-1)15-19-11-13-20(14-12-19)16-18-9-5-2-6-10-18/h1-10,
InchiKey:	XUABFDHAIDJKOQ-UHFFFAOYSA-N
Formula:	C20H24
SMILES:	<chem>c1ccc(CC2CCC(Cc3ccccc3)CC2)cc1</chem>
Mol. weight [g/mol]:	264.40
CAS:	128484-66-2

Physical Properties

Property code	Value	Unit	Source
affp	805.70	kJ/mol	NIST Webbook
basg	773.30	kJ/mol	NIST Webbook
gf	359.08	kJ/mol	Joback Method
hf	50.91	kJ/mol	Joback Method
hfus	28.54	kJ/mol	Joback Method
hvap	64.79	kJ/mol	Joback Method
log10ws	-5.81		Crippen Method
logp	5.278		Crippen Method
mcvol	234.280	ml/mol	McGowan Method
pc	1883.80	kPa	Joback Method
tb	725.24	K	Joback Method
tc	974.70	K	Joback Method
tf	371.14	K	Joback Method
vc	0.872	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	685.68	J/mol×K	725.24	Joback Method
cpg	783.02	J/mol×K	933.12	Joback Method
cpg	766.95	J/mol×K	891.54	Joback Method
cpg	749.29	J/mol×K	849.97	Joback Method
cpg	729.94	J/mol×K	808.39	Joback Method
cpg	708.77	J/mol×K	766.82	Joback Method
cpg	797.62	J/mol×K	974.70	Joback Method

dvisc	0.0001282	Pa×s	725.24	Joback Method
dvisc	0.0001665	Pa×s	666.22	Joback Method
dvisc	0.0002274	Pa×s	607.21	Joback Method
dvisc	0.0003321	Pa×s	548.19	Joback Method
dvisc	0.0005315	Pa×s	489.17	Joback Method
dvisc	0.0009679	Pa×s	430.16	Joback Method
dvisc	0.0021326	Pa×s	371.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C128484662&Units=SI
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

Legend

affp:	Proton affinity
basg:	Gas basicity
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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