

2,2 Bis(p-allyloxy phenyl) butane

Inchi:	InChI=1S/C22H26O2/c1-5-16-23-20-12-8-18(9-13-20)22(4,7-3)19-10-14-21(15-11-19)24
InchiKey:	UASXNVYMDZGKGU-UHFFFAOYSA-N
Formula:	C22H26O2
SMILES:	C=CCOc1ccc(C(C)(CC)c2ccc(OCC=C)cc2)cc1
Mol. weight [g/mol]:	322.44
CAS:	116346-12-4

Physical Properties

Property code	Value	Unit	Source
gf	308.44	kJ/mol	Joback Method
hf	-69.62	kJ/mol	Joback Method
hfus	32.44	kJ/mol	Joback Method
hvap	72.63	kJ/mol	Joback Method
log10ws	-6.12		Crippen Method
logp	5.532		Crippen Method
mvol	276.460	ml/mol	McGowan Method
pc	1446.83	kPa	Joback Method
tb	801.05	K	Joback Method
tc	1024.13	K	Joback Method
tf	458.94	K	Joback Method
vc	1.038	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	811.31	J/molxK	801.05	Joback Method
cpg	829.15	J/molxK	838.23	Joback Method
cpg	845.70	J/molxK	875.41	Joback Method
cpg	861.02	J/molxK	912.59	Joback Method
cpg	875.19	J/molxK	949.77	Joback Method
cpg	888.29	J/molxK	986.95	Joback Method
cpg	900.39	J/molxK	1024.13	Joback Method
dvisc	0.0005149	Paxs	458.94	Joback Method
dvisc	0.0002687	Paxs	515.96	Joback Method

dvisc	0.0001596	Paxs	572.98	Joback Method
dvisc	0.0001042	Paxs	630.00	Joback Method
dvisc	0.0000730	Paxs	687.01	Joback Method
dvisc	0.0000540	Paxs	744.03	Joback Method
dvisc	0.0000417	Paxs	801.05	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346124&Units=SI

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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