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
hfus	32.44	kJ/mol	Joback Method
logp	5.532		Crippen Method
mcvol	276.460	ml/mol	McGowan Method
tb	680.51	K	Cheméo Relay (1.0)

Correlations

Information	Value
Property code	cpg
Equation	Y = A + B·T + C·T² + D·T³ + E·T.
Y unit	J/mol×K
Coeff. A	-3.57770e+01
Coeff. B	1.77644e+00
Coeff. C	-1.09692e-03
Coeff. D	2.48900e-07
Coeff. E	0.00000e+00
Basis	predicted
Temperature range (K), min.	273.00
Temperature range (K), max.	1000.00

Information	Value
Property code	dvisc
Equation	Y = exp(A + B/T + C·ln(T) + D·T^E)
Y unit	Pa×s

Coeff. A	-1.34561e+01
Coeff. B	2.70068e+03
Coeff. C	0.00000e+00
Coeff. D	0.00000e+00
Coeff. E	0.00000e+00
Basis	predicted
Comment	Liquid phase. Joback/Reid (1987), valid from Tf to 0.7·Tc.
Temperature range (K), min.	458.94
Temperature range (K), max.	717.07

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116346124&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hfus:	Enthalpy of fusion at standard conditions
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature

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