

11-(4-Methoxyphenyl)-6,11-dihydrodibenzo[b,e]ox

Inchi:	InChI=1S/C21H18O3/c1-23-17-12-10-16(11-13-17)21(22)18-7-3-2-6-15(18)14-24-20-9-5
InchiKey:	HUFIZHPVTCKYGH-UHFFFAOYSA-N
Formula:	C21H18O3
SMILES:	<chem>COc1ccc(C2(O)c3ccccc3COc3ccccc32)cc1</chem>
Mol. weight [g/mol]:	318.37

Physical Properties

Property code	Value	Unit	Source
gf	161.60	kJ/mol	Joback Method
hf	-130.00	kJ/mol	Joback Method
hfus	36.19	kJ/mol	Joback Method
hvap	93.52	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	3.872		Crippen Method
mcvol	242.220	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2653.00		NIST Webbook
ripol	3649.00		NIST Webbook
ripol	3649.00		NIST Webbook
tb	923.39	K	Joback Method
tc	1171.60	K	Joback Method
tf	594.71	K	Joback Method
vc	0.900	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	750.79	J/molxK	923.39	Joback Method
cpg	767.51	J/molxK	964.76	Joback Method
cpg	784.30	J/molxK	1006.13	Joback Method
cpg	801.42	J/molxK	1047.50	Joback Method
cpg	819.10	J/molxK	1088.86	Joback Method
cpg	837.60	J/molxK	1130.23	Joback Method
cpg	857.17	J/molxK	1171.60	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=R537672&Units=SI

Legend

cpg:	Ideal gas heat capacity
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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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