

4,4'-Bis(fluorophenyl)ether

Other names:	1,1'-oxybis(4-fluorobenzene) 4-Fluorophenyl ether Benzene, 1,1'-oxybis[4-fluoro- Bis(p-fluorophenyl) ether
Inchi:	InChI=1S/C12H8F2O/c13-9-1-5-11(6-2-9)15-12-7-3-10(14)4-8-12/h1-8H
InchiKey:	UUKHFGSOCZLVJO-UHFFFAOYSA-N
Formula:	C12H8F2O
SMILES:	Fc1ccc(Oc2ccc(F)cc2)cc1
Mol. weight [g/mol]:	206.19

Physical Properties

Property code	Value	Unit	Source
af	0.5015		Cheméo Relay (1.0)
gf	-238.90	kJ/mol	Joback Method
hf	-326.99	kJ/mol	Cheméo Relay (1.0)
hfus	21.49	kJ/mol	Joback Method
hvap	68.20	kJ/mol	Cheméo Relay (1.0)
ie	8.11	eV	Cheméo Relay (1.0)
log10ws	-4.63		Cheméo Relay (1.0)
logp	3.757		Crippen Method
mcvol	141.830	ml/mol	McGowan Method
pc	2937.70	kPa	Joback Method
tb	534.88	K	Cheméo Relay (1.0)
tc	772.87	K	Cheméo Relay (1.0)
tf	312.32	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.55	J/mol×K	558.24	Joback Method
cpg	332.10	J/mol×K	595.52	Joback Method
cpg	344.77	J/mol×K	632.79	Joback Method
cpg	356.58	J/mol×K	670.07	Joback Method
cpg	367.55	J/mol×K	707.34	Joback Method

cpg	377.72	J/mol×K	744.62	Joback Method
cpg	387.11	J/mol×K	781.89	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C330938&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.cheméo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

af:	Acentric Factor
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
ie:	Ionization energy
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

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