Bis[4-(1,1,3,3-tetramethylbutyl)phenyl] ether

Other names: Benzene, 1,1'-oxy-, bis[4-(1,1,3,3-tetramethylbutyl)]-
Inchi: InChI=1S/C28H42O/c1-25(2,3)19-27(7,8)21-11-15-23(16-12-21)29-24-17-13-22(14-18-24
InchiKey: AJDONJVWDSZZQF-UHFFFAOYSA-N
Formula: C28H42O
SMILES: CC(C)(C)CC(C)(C)c1ccc(Oc2ccc(C(C)(C)CC(C)(C)C)cc2)cc1
Mol. weight [g/mol]: 394.63
CAS: 101-58-6

Physical Properties

Property code	Value	Unit	Source
gf	296.80	kJ/mol	Joback Method
hf	-338.35	kJ/mol	Joback Method
hfus	27.11	kJ/mol	Joback Method
hvap	81.02	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	8.906		Crippen Method
mcvol	363.730	ml/mol	McGowan Method
pc	967.47	kPa	Joback Method
tb	912.86	K	Joback Method
tc	1144.00	K	Joback Method
tf	515.11	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1199.72	J/mol×K	912.86	Joback Method
cpg	1220.56	J/mol×K	951.38	Joback Method
cpg	1240.16	J/mol×K	989.91	Joback Method
cpg	1258.71	J/mol×K	1028.43	Joback Method
cpg	1276.40	J/mol×K	1066.95	Joback Method
cpg	1293.43	J/mol×K	1105.48	Joback Method
cpg	1309.99	J/mol×K	1144.00	Joback Method
dvisc	0.0002798	Pa×s	515.11	Joback Method

dvisc	0.0001155	Pa×s	581.40	Joback Method
dvisc	0.0000572	Pa×s	647.69	Joback Method
dvisc	0.0000323	Pa×s	713.98	Joback Method
dvisc	0.0000200	Pa×s	780.28	Joback Method
dvisc	0.0000134	Pa×s	846.57	Joback Method
dvisc	0.0000095	Pa×s	912.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C101586&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

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