Benzene, 1,3-bis(1,1-dimethylethyl)-2-methoxy-5-methyl-

Other names: 2,6-bis-(tertiobutyl)-4-methyl anisole
Inchi: InChI=1S/C16H26O/c1-11-9-12(15(2,3)4)14(17-8)13(10-11)16(5,6)7/h9-10H,1-8H3
InchiKey: TVWAVADIILZVIY-UHFFFAOYSA-N
Formula: C16H26O
SMILES: COc1c(C(C)(C)C)cc(C)cc1C(C)(C)C
Mol. weight [g/mol]: 234.38
CAS: 1518-53-2

Physical Properties

Property code	Value	Unit	Source
gf	68.04	kJ/mol	Joback Method
hf	-321.17	kJ/mol	Joback Method
hfus	16.43	kJ/mol	Joback Method
hvap	55.29	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.599		Crippen Method
mcvol	218.410	ml/mol	McGowan Method
pc	1670.06	kPa	Joback Method
rinpol	1496.00		NIST Webbook
rinpol	1496.00		NIST Webbook
tb	623.06	K	Joback Method
tc	835.09	K	Joback Method
tf	361.13	K	Joback Method
vc	0.820	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	580.40	J/mol×K	623.06	Joback Method
cpg	667.94	J/mol×K	799.75	Joback Method
cpg	652.58	J/mol×K	764.41	Joback Method
cpg	636.21	J/mol×K	729.07	Joback Method
cpg	618.76	J/mol×K	693.74	Joback Method
cpg	600.17	J/mol×K	658.40	Joback Method

cpg	682.34	J/mol×K	835.09	Joback Method
dvisc	0.0000884	Pa×s	623.06	Joback Method
dvisc	0.0001167	Pa×s	579.40	Joback Method
dvisc	0.0001613	Pa×s	535.75	Joback Method
dvisc	0.0002360	Pa×s	492.09	Joback Method
dvisc	0.0003720	Pa×s	448.44	Joback Method
dvisc	0.0006468	Pa×s	404.78	Joback Method
dvisc	0.0012854	Pa×s	361.13	Joback Method

Sources

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=C1518532&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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