4-(1,1,3,3-Tetramethylbutyl)phenyl-3,6-dimethyl-1-ether

InChI: InChI=1S/C22H34O/c1-16-8-9-17(2)20(14-16)23-19-12-10-18(11-13-19)22(6,7)15-21(3,4

InChIKey: SOPYOYMCUZNUBV-UHFFFAOYSA-N

Formula: C22H34O

SMILES: CC1C=C(Oc2ccc(C(C)(C)CC(C)(C)C)cc2)C(C)CC1

Mol. weight [g/mol]: 314.50

Physical Properties

Property code	Value	Unit	Source
gf	174.89	kJ/mol	Joback Method
hf	-341.78	kJ/mol	Joback Method
hfus	26.49	kJ/mol	Joback Method
hvap	68.40	kJ/mol	Joback Method
log10ws	-7.03		Crippen Method
logp	6.729		Crippen Method
mcvol	287.790	ml/mol	McGowan Method
pc	1275.51	kPa	Joback Method
ripol	3005.00		NIST Webbook
tb	769.40	K	Joback Method
tc	993.79	K	Joback Method
tf	420.13	K	Joback Method
vc	1.073	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	894.73	J/mol×K	769.40	Joback Method
cpg	917.59	J/mol×K	806.80	Joback Method
cpg	938.80	J/mol×K	844.20	Joback Method
cpg	958.47	J/mol×K	881.60	Joback Method
cpg	976.68	J/mol×K	919.00	Joback Method
cpg	993.53	J/mol×K	956.39	Joback Method
cpg	1009.12	J/mol×K	993.79	Joback Method
dvisc	0.0010039	Pa×s	420.13	Joback Method
dvisc	0.0004596	Pa×s	478.34	Joback Method

dvisc	0.0002493	Pa×s	536.55	Joback Method
dvisc	0.0001525	Pa×s	594.76	Joback Method
dvisc	0.0001018	Pa×s	652.98	Joback Method
dvisc	0.0000726	Pa×s	711.19	Joback Method
dvisc	0.0000545	Pa×s	769.40	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R58511&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume