

4-(1,1,3,3-Tetramethylbutyl)phenyl-3-methyl-1,3-butadiene

InChI:
InChIKey:

InChI=1S/C19H28O/c1-15(2)12-13-20-17-10-8-16(9-11-17)19(6,7)14-18(3,4)5/h8-13H,1,

FTDKMGTYCVOHRR-OUKQBFOZSA-N

Formula:

C19H28O

SMILES:

C=C(C)C=COc1ccc(C(C)(C)CC(C)(C)C)cc1

Mol. weight [g/mol]:

272.43

Physical Properties

Property code	Value	Unit	Source
gf	272.07	kJ/mol	Joback Method
hf	-127.29	kJ/mol	Joback Method
hfus	22.59	kJ/mol	Joback Method
hvap	60.01	kJ/mol	Joback Method
log10ws	-6.21		Crippen Method
logp	5.869		Crippen Method
mcvol	252.080	ml/mol	McGowan Method
pc	1472.49	kPa	Joback Method
ripol	2546.00		NIST Webbook
ripol	2546.00		NIST Webbook
tb	682.46	K	Joback Method
tc	898.12	K	Joback Method
tf	349.10	K	Joback Method
vc	0.950	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.50	J/mol×K	682.46	Joback Method
cpg	719.71	J/mol×K	718.40	Joback Method
cpg	738.59	J/mol×K	754.35	Joback Method
cpg	756.23	J/mol×K	790.29	Joback Method
cpg	772.75	J/mol×K	826.23	Joback Method
cpg	788.25	J/mol×K	862.18	Joback Method
cpg	802.83	J/mol×K	898.12	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R316480&Units=SI
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

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
hvp:	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
ripl:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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