

Carvacrol methyl ether

Other names:	Methyl carvacrol Carvacryl methyl oxide Carvacryl methyl ether Carvacrol Me ether methyl-ether Carvacrol Carvacrol methyl 5-Isopropyl-2-methylanisole
Inchi:	InChI=1S/C11H16O/c1-8(2)10-6-5-9(3)11(7-10)12-4/h5-8H,1-4H3
InchiKey:	YVLHTQPPMZOCOW-UHFFFAOYSA-N
Formula:	C11H16O
SMILES:	COc1cc(C(C)C)ccc1C
Mol. weight [g/mol]:	164.24
CAS:	6379-73-3

Physical Properties

Property code	Value	Unit	Source
gf	27.45	kJ/mol	Joback Method
hf	-194.28	kJ/mol	Joback Method
hfus	15.17	kJ/mol	Joback Method
hvap	45.70	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.127		Crippen Method
mcvol	147.960	ml/mol	McGowan Method
pc	2545.61	kPa	Joback Method
rinpol	1225.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1244.00		NIST Webbook
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ripol	1595.00		NIST Webbook
ripol	1614.00		NIST Webbook
tb	509.70	K	Joback Method
tc	716.96	K	Joback Method
tf	272.42	K	Joback Method
vc	0.555	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.70	J/mol×K	509.70	Joback Method
cpg	396.29	J/mol×K	682.41	Joback Method
cpg	383.76	J/mol×K	647.87	Joback Method
cpg	370.54	J/mol×K	613.33	Joback Method
cpg	356.63	J/mol×K	578.79	Joback Method
cpg	342.03	J/mol×K	544.24	Joback Method
cpg	408.15	J/mol×K	716.96	Joback Method
dvisc	0.0001623	Pa×s	509.70	Joback Method
dvisc	0.0002057	Pa×s	470.15	Joback Method
dvisc	0.0002723	Pa×s	430.61	Joback Method
dvisc	0.0003817	Pa×s	391.06	Joback Method
dvisc	0.0005771	Pa×s	351.51	Joback Method
dvisc	0.0009689	Pa×s	311.97	Joback Method
dvisc	0.0018910	Pa×s	272.42	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6379733&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

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

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