

o-Cresol, isoBOC

Inchi:	InChI=1S/C12H16O3/c1-9(2)8-14-12(13)15-11-7-5-4-6-10(11)3/h4-7,9H,8H2,1-3H3
InchiKey:	LLXWOUNCYHNMCV-UHFFFAOYSA-N
Formula:	C12H16O3
SMILES:	Cc1ccccc1OC(=O)OCC(C)C
Mol. weight [g/mol]:	208.25

Physical Properties

Property code	Value	Unit	Source
gf	-188.42	kJ/mol	Joback Method
hf	-448.25	kJ/mol	Joback Method
hfus	20.94	kJ/mol	Joback Method
hvap	56.42	kJ/mol	Joback Method
log10ws	-3.34		Crippen Method
logp	3.166		Crippen Method
mvol	169.490	ml/mol	McGowan Method
pc	2458.04	kPa	Joback Method
rinpol	1446.00		NIST Webbook
rinpol	1446.00		NIST Webbook
tb	603.89	K	Joback Method
tc	812.91	K	Joback Method
tf	343.33	K	Joback Method
vc	0.635	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.73	J/molxK	603.89	Joback Method
cpg	486.66	J/molxK	778.07	Joback Method
cpg	474.87	J/molxK	743.24	Joback Method
cpg	462.28	J/molxK	708.40	Joback Method
cpg	448.90	J/molxK	673.56	Joback Method
cpg	434.72	J/molxK	638.73	Joback Method
cpg	497.67	J/molxK	812.91	Joback Method
dvisc	0.0001353	Paxs	603.89	Joback Method

dvisc	0.0001738	Paxs	560.46	Joback Method
dvisc	0.0002328	Paxs	517.04	Joback Method
dvisc	0.0003290	Paxs	473.61	Joback Method
dvisc	0.0004986	Paxs	430.18	Joback Method
dvisc	0.0008297	Paxs	386.76	Joback Method
dvisc	0.0015703	Paxs	343.33	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R235306&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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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

Latest version available from:

<https://www.chemeo.com/cid/57-508-5/o-Cresol-isoBOC.pdf>

Generated by Cheméo on 2024-04-17 01:46:21.133671916 +0000 UTC m=+15607630.054249228.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.