

# O-cresol, 4-bromo-alpha,alpha,alpha-trifluoro-

<b>Inchi:</b>	InChI=1S/C7H4BrF3O/c8-4-1-2-6(12)5(3-4)7(9,10)11/h1-3,12H
<b>InchiKey:</b>	PDPGERGWEOJVDU-UHFFFAOYSA-N
<b>Formula:</b>	C7H4BrF3O
<b>SMILES:</b>	Oc1ccc(Br)cc1C(F)(F)F
<b>Mol. weight [g/mol]:</b>	241.00
<b>CAS:</b>	50824-04-9

## Physical Properties

Property code	Value	Unit	Source
gf	-611.05	kJ/mol	Joback Method
hf	-710.81	kJ/mol	Joback Method
hfus	20.43	kJ/mol	Joback Method
hvap	49.82	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.173		Crippen Method
mvol	114.410	ml/mol	McGowan Method
pc	4615.13	kPa	Joback Method
tb	532.58	K	Joback Method
tc	757.84	K	Joback Method
tf	383.30	K	Joback Method
vc	0.391	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.90	J/molxK	532.58	Joback Method
cpg	252.34	J/molxK	570.12	Joback Method
cpg	259.92	J/molxK	607.67	Joback Method
cpg	266.73	J/molxK	645.21	Joback Method
cpg	272.88	J/molxK	682.75	Joback Method
cpg	278.48	J/molxK	720.29	Joback Method
cpg	283.63	J/molxK	757.84	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C50824049&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50824049&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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