

# 4-(Trifluoromethoxy)benzyl bromide

<b>Inchi:</b>	InChI=1S/C8H6BrF3O/c9-5-6-1-3-7(4-2-6)13-8(10,11)12/h1-4H,5H2
<b>InchiKey:</b>	JDNPUJCKXLOHOW-UHFFFAOYSA-N
<b>Formula:</b>	C8H6BrF3O
<b>SMILES:</b>	FC(F)(F)Oc1ccc(CBr)cc1
<b>Mol. weight [g/mol]:</b>	255.03
<b>CAS:</b>	50824-05-0

## Physical Properties

Property code	Value	Unit	Source
gf	-553.01	kJ/mol	Joback Method
hf	-686.36	kJ/mol	Joback Method
hfus	18.43	kJ/mol	Joback Method
hvap	41.44	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.480		Crippen Method
mcvol	128.500	ml/mol	McGowan Method
pc	3325.84	kPa	Joback Method
tb	497.26	K	Joback Method
tc	703.82	K	Joback Method
tf	305.08	K	Joback Method
vc	0.498	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	263.26	J/molxK	497.26	Joback Method
cpg	273.92	J/molxK	531.69	Joback Method
cpg	283.84	J/molxK	566.11	Joback Method
cpg	293.06	J/molxK	600.54	Joback Method
cpg	301.60	J/molxK	634.97	Joback Method
cpg	309.52	J/molxK	669.39	Joback Method
cpg	316.84	J/molxK	703.82	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C50824050&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C50824050&amp;Units=SI</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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