

Benzene, 1-bromo-4-(trifluoromethyl)-

Other names:	Toluene, p-bromo-«alpha», «alpha», «alpha»-trifluoro-p-(Trifluoromethyl)bromobenzene p-Bromo-«alpha», «alpha», «alpha»-trifluorotoluene p-Bromobenzotrifluoride para-Bromobenzotrifluoride 1-Bromo-4-(trifluoromethyl)benzene 4-Bromobenzotrifluoride 4-Trifluoromethylbromobenzene 4-Bromo-«alpha», «alpha», «alpha»-trifluorotoluene
Inchi:	InChI=1S/C7H4BrF3/c8-6-3-1-5(2-4-6)7(9,10)11/h1-4H
InchiKey:	XLQSXGGDTHANLN-UHFFFAOYSA-N
Formula:	C7H4BrF3
SMILES:	FC(F)(F)c1ccc(Br)cc1
Mol. weight [g/mol]:	225.01
CAS:	402-43-7

Physical Properties

Property code	Value	Unit	Source
gf	-456.43	kJ/mol	Joback Method
hf	-533.50	kJ/mol	Joback Method
hfus	14.65	kJ/mol	Joback Method
hvap	36.80	kJ/mol	Joback Method
ie	9.48	eV	NIST Webbook
ie	9.55	eV	NIST Webbook
log10ws	-3.74		Crippen Method
logp	3.468		Crippen Method
mcvol	108.540	ml/mol	McGowan Method
pc	3805.69	kPa	Joback Method
rinpol	916.10		NIST Webbook
rinpol	916.10		NIST Webbook
rinpol	916.10		NIST Webbook
tb	427.50 ± 0.50	K	NIST Webbook
tb	427.50 ± 0.50	K	NIST Webbook
tb	427.70	K	NIST Webbook
tc	663.16	K	Joback Method
tf	271.58	K	Joback Method
vc	0.424	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	201.47	J/mol×K	451.96	Joback Method
cpg	211.43	J/mol×K	487.16	Joback Method
cpg	220.58	J/mol×K	522.36	Joback Method
cpg	228.96	J/mol×K	557.56	Joback Method
cpg	236.64	J/mol×K	592.76	Joback Method
cpg	243.66	J/mol×K	627.96	Joback Method
cpg	250.07	J/mol×K	663.16	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C402437&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume

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