

Benzene, 1-(bromomethyl)-3-fluoro-

Other names:	Toluene, «alpha»-bromo-m-fluoro-m-Fluorobenzylbromide 3-Fluorobenzyl bromide meta-Fluorobenzyl bromide «alpha»-Bromo-3-fluorotoluene «alpha»-bromo-m-fluorotoluene
Inchi:	InChI=1S/C7H6BrF/c8-5-6-2-1-3-7(9)4-6/h1-4H,5H2
InchiKey:	SCBZBMXPJYMXRC-UHFFFAOYSA-N
Formula:	C7H6BrF
SMILES:	Fc1cccc(CBr)c1
Mol. weight [g/mol]:	189.03
CAS:	456-41-7

Physical Properties

Property code	Value	Unit	Source
gf	-69.65	kJ/mol	Joback Method
hf	-132.53	kJ/mol	Joback Method
hfus	15.90	kJ/mol	Joback Method
hvap	39.73	kJ/mol	Joback Method
log10ws	-3.11		Crippen Method
logp	2.721		Crippen Method
mcvol	105.000	ml/mol	McGowan Method
pc	4162.33	kPa	Joback Method
tb	456.65	K	Joback Method
tc	677.45	K	Joback Method
tf	267.98	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	181.66	J/mol×K	456.65	Joback Method
cpg	191.53	J/mol×K	493.45	Joback Method
cpg	200.73	J/mol×K	530.25	Joback Method

cpg	209.31	J/mol×K	567.05	Joback Method
cpg	217.30	J/mol×K	603.85	Joback Method
cpg	224.74	J/mol×K	640.65	Joback Method
cpg	231.65	J/mol×K	677.45	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	361.20	K	2.70	NIST Webbook

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=C456417&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:

<https://www.cheméo.com/cid/66-088-2/Benzene-1-bromomethyl-3-fluoro.pdf>

Generated by Cheméo on 2025-12-05 15:52:02.363196653 +0000 UTC m=+4698119.893237317.

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