3-FLUOROBENZAL BROMIDE

Other names:	3-Fluorobenzal bromide
	meta-(Dibromomethyl)fluorobenzene
	Benzene, 1-(dibromomethyl)-3-fluoro-
	3-bromobenzal bromide
Inchi:	InChI=1S/C7H5Br2F/c8-7(9)5-2-1-3-6(10)4-5/h1-4,7H
InchiKey:	ZIAHZFPHXNQNQN-UHFFFAOYSA-N
Formula:	C7H5Br2F
SMILES:	Fc1cccc(C(Br)Br)c1
Mol. weight [g/mol]:	267.92

Physical Properties

Property code	Value	Unit	Source
hf	-76.25	kJ/mol	Cheméo Relay (1.0)
hfus	17.67	kJ/mol	Joback Method
hvap	60.78	kJ/mol	Cheméo Relay (1.0)
ie	9.39	eV	Cheméo Relay (1.0)
log10ws	-3.21		Cheméo Relay (1.0)
logp	3.614		Crippen Method
mcvol	122.500	ml/mol	McGowan Method
tb	480.63	K	Cheméo Relay (1.0)
tf	298.34	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.79	J/mol×K	522.37	Joback Method
cpg	222.07	J/mol×K	562.94	Joback Method
cpg	230.57	J/mol×K	603.52	Joback Method
cpg	238.35	J/mol×K	644.09	Joback Method
cpg	245.46	J/mol×K	684.66	Joback Method
cpg	251.97	J/mol×K	725.23	Joback Method
cpg	257.94	J/mol×K	765.81	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	382.20	K	1.00	NIST Webbook

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C455345&Units=SI

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Legend

cpg: Ideal gas heat capacity

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

tb: Normal Boiling Point Temperature

tbrp: Boiling point at reduced pressure

tf: Normal melting (fusion) point