Fluorobenzene, meta-(dibromomethyl)-

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
CAS:	455-34-5

Physical Properties

Property code	Value	Unit	Source
gf	-57.77	kJ/mol	Joback Method
hf	-111.48	kJ/mol	Joback Method
hfus	17.67	kJ/mol	Joback Method
hvap	45.78	kJ/mol	Joback Method
log10ws	-4.00		Crippen Method
logp	3.614		Crippen Method
mcvol	122.500	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	522.37	K	Joback Method
tc	765.81	K	Joback Method
tf	312.78	K	Joback Method
vc	0.456	m3/kmol	Joback Method

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

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C455345&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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