2,5-Difluorobenzylbromide

Other names:	Benzene, 2-(bromomethyl)-1,4-difluoro- 2-(bromomethyl)-1,4-difluorobenzene
Inchi:	InChI=1S/C7H5BrF2/c8-4-5-3-6(9)1-2-7(5)10/h1-3H,4H2
InchiKey:	ONWGSWNHQZYCFK-UHFFFAOYSA-N
Formula:	C7H5BrF2
SMILES:	Fc1ccc(F)c(CBr)c1
Mol. weight [g/mol]:	207.02

Physical Properties

Property code	Value	Unit	Source
hfus	18.59	kJ/mol	Joback Method
hvap	54.56	kJ/mol	Cheméo Relay (1.0)
ie	9.17	eV	Cheméo Relay (1.0)
logp	2.860		Crippen Method
mcvol	106.770	ml/mol	McGowan Method
tb	465.83	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	190.11	J/mol×K	460.90	Joback Method
cpg	199.00	J/mol×K	495.93	Joback Method
cpg	207.35	J/mol×K	530.97	Joback Method
cpg	215.19	J/mol×K	566.00	Joback Method
cpg	222.54	J/mol×K	601.04	Joback Method
cpg	229.41	J/mol×K	636.07	Joback Method
cpg	235.85	J/mol×K	671.11	Joback Method

Sources

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

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C85117993&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

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature