

1-Bromo-1,1-difluoroethane

Inchi:	InChI=1S/C2H3BrF2/c1-2(3,4)5/h1H3
InchiKey:	MGCGGCMKJWCMKL-UHFFFAOYSA-N
Formula:	C2H3BrF2
SMILES:	CC(F)(F)Br
Mol. weight [g/mol]:	144.95
CAS:	420-47-3

Physical Properties

Property code	Value	Unit	Source
gf	-406.50	kJ/mol	Joback Method
hf	-474.30 ± 8.50	kJ/mol	NIST Webbook
hfus	4.97	kJ/mol	Joback Method
hvap	23.55	kJ/mol	Joback Method
log10ws	-1.90		Crippen Method
logp	1.994		Crippen Method
mcvol	60.080	ml/mol	McGowan Method
pc	5015.69	kPa	Joback Method
tb	306.63	K	Joback Method
tc	482.76	K	Joback Method
tf	175.70	K	Joback Method
vc	0.234	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	83.73	J/molxK	306.63	Joback Method
cpg	89.29	J/molxK	335.99	Joback Method
cpg	94.46	J/molxK	365.34	Joback Method
cpg	99.26	J/molxK	394.70	Joback Method
cpg	103.69	J/molxK	424.05	Joback Method
cpg	107.79	J/molxK	453.41	Joback Method
cpg	111.57	J/molxK	482.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C420473&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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

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
mccvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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