

Ethane, 1-bromo-1,1,2,2-tetrafluoro-2-iodo-

Other names:	1-Bromo-2-iodotetrafluoroethane 1-bromotetrafluoro-2-iodoethane
Inchi:	InChI=1S/C2BrF4I/c3-1(4,5)2(6,7)8
InchiKey:	ZYNPYKGTNSXKPI-UHFFFAOYSA-N
Formula:	C2BrF4I
SMILES:	FC(F)(Br)C(F)(F)I
Mol. weight [g/mol]:	306.82
CAS:	421-70-5

Physical Properties

Property code	Value	Unit	Source
gf	-735.16	kJ/mol	Joback Method
hf	-783.35	kJ/mol	Joback Method
hfus	8.12	kJ/mol	Joback Method
hvap	29.99	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.002		Crippen Method
mvol	89.440	ml/mol	McGowan Method
pc	4414.96	kPa	Joback Method
tb	351.00	K	NIST Webbook
tc	604.93	K	Joback Method
tf	237.36	K	Joback Method
vc	0.347	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.09	J/molxK	395.08	Joback Method
cpg	141.86	J/molxK	430.05	Joback Method
cpg	146.85	J/molxK	465.03	Joback Method
cpg	151.12	J/molxK	500.00	Joback Method
cpg	154.73	J/molxK	534.98	Joback Method
cpg	157.76	J/molxK	569.95	Joback Method
cpg	160.26	J/molxK	604.93	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=C421705&Units=SI

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
h vap:	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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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