1,1-Difluoro-1-iodoethane

Inchi: InChI=1S/C2H3F2I/c1-2(3,4)5/h1H3
InchiKey: LBRHUMBEGYYRBE-UHFFFAOYSA-N
Formula: C2H3F2I
SMILES: CC(F)(F)I
Mol. weight [g/mol]: 191.95
CAS: 598-39-0

Physical Properties

Property code	Value	Unit	Source
gf	-362.70	kJ/mol	Joback Method
hf	-410.00 ± 8.50	kJ/mol	NIST Webbook
hfus	4.09	kJ/mol	Joback Method
hvap	26.49	kJ/mol	Joback Method
log10ws	-2.42		Crippen Method
logp	2.034		Crippen Method
mcvol	68.400	ml/mol	McGowan Method
pc	4426.72	kPa	Joback Method
tb	333.61	K	Joback Method
tc	529.90	K	Joback Method
tf	173.96	K	Joback Method
vc	0.261	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	91.73	J/mol×K	333.61	Joback Method
cpg	97.37	J/mol×K	366.32	Joback Method
cpg	102.53	J/mol×K	399.04	Joback Method
cpg	107.25	J/mol×K	431.75	Joback Method
cpg	111.55	J/mol×K	464.47	Joback Method
cpg	115.46	J/mol×K	497.18	Joback Method
cpg	119.01	J/mol×K	529.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C598390&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume