1,3-Butadiyne, 1,4-difluoro-

Inchi: InChI=1S/C4F2/c5-3-1-2-4-6
InchiKey: XOQUBARPWKCNSI-UHFFFAOYSA-N
Formula: C4F2
SMILES: FC#CC#CF
Mol. weight [g/mol]: 86.04
CAS: 64788-23-4

Physical Properties

Property code	Value	Unit	Source
gf	-1.22	kJ/mol	Joback Method
hf	26.49	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	27.17	kJ/mol	Joback Method
ie	10.05	eV	NIST Webbook
ie	10.35	eV	NIST Webbook
log10ws	-1.78		Crippen Method
logp	0.847		Crippen Method
mcvol	53.560	ml/mol	McGowan Method
pc	5312.41	kPa	Joback Method
tb	307.46	K	Joback Method
tc	502.20	K	Joback Method
tf	348.22	K	Joback Method
vc	0.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	75.86	J/mol×K	307.46	Joback Method
cpg	78.52	J/mol×K	339.92	Joback Method
cpg	81.11	J/mol×K	372.37	Joback Method
cpg	83.62	J/mol×K	404.83	Joback Method
cpg	86.06	J/mol×K	437.28	Joback Method
cpg	88.43	J/mol×K	469.74	Joback Method
cpg	90.72	J/mol×K	502.20	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C64788234&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
ie:	Ionization energy
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