Bicyclo[4.1.0]hepta-1,3,5-triene, 7,7-difluoro-

Other names: 1,1-Difluoro-cyclopropabenzene
Inchi: InChI=1S/C7H4F2/c8-7(9)5-3-1-2-4-6(5)7/h1-4H
InchiKey: QQESEAYTNOTARV-UHFFFAOYSA-N
Formula: C7H4F2
SMILES: FC1(F)c2ccccc21
Mol. weight [g/mol]: 126.10
CAS: 18238-55-6

Physical Properties

Property code	Value	Unit	Source
gf	-199.32	kJ/mol	Joback Method
hf	-254.61	kJ/mol	Joback Method
hfus	9.73	kJ/mol	Joback Method
hvap	30.90	kJ/mol	Joback Method
ie	10.10	eV	NIST Webbook
log10ws	-2.19		Crippen Method
logp	2.140		Crippen Method
mcvol	78.410	ml/mol	McGowan Method
pc	4222.04	kPa	Joback Method
tb	388.20	K	Joback Method
tc	587.28	K	Joback Method
tf	257.65	K	Joback Method
vc	0.327	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	144.40	J/mol×K	388.20	Joback Method
cpg	154.71	J/mol×K	421.38	Joback Method
cpg	163.90	J/mol×K	454.56	Joback Method
cpg	172.06	J/mol×K	487.74	Joback Method
cpg	179.33	J/mol×K	520.92	Joback Method
cpg	185.81	J/mol×K	554.10	Joback Method
cpg	191.64	J/mol×K	587.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C18238556&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