1,1'-Biphenyl,3,3'-difluoro-

Other names: 3,3'-difluoro-1,1'-biphenyl
Inchi: InChI=1S/C12H8F2/c13-11-5-1-3-9(7-11)10-4-2-6-12(14)8-10/h1-8H
InchiKey: GAYJHUJLHJWCTH-UHFFFAOYSA-N
Formula: C12H8F2
SMILES: Fc1cccc(-c2cccc(F)c2)c1
Mol. weight [g/mol]: 190.19
CAS: 396-64-5

Physical Properties

Property code	Value	Unit	Source
gf	-133.90	kJ/mol	Joback Method
hf	-233.11	kJ/mol	Joback Method
hfus	20.30	kJ/mol	Joback Method
hvap	46.55	kJ/mol	Joback Method
ie	8.35 ± 0.02	eV	NIST Webbook
log10ws	-4.74		Crippen Method
logp	3.632		Crippen Method
mcvol	135.960	ml/mol	McGowan Method
pc	2992.59	kPa	Joback Method
tb	535.82	K	Joback Method
tc	762.30	K	Joback Method
tf	304.06	K	Joback Method
vc	0.527	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.88	J/mol×K	535.82	Joback Method
cpg	308.80	J/mol×K	573.57	Joback Method
cpg	321.75	J/mol×K	611.31	Joback Method
cpg	333.77	J/mol×K	649.06	Joback Method
cpg	344.91	J/mol×K	686.81	Joback Method
cpg	355.21	J/mol×K	724.55	Joback Method
cpg	364.72	J/mol×K	762.30	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	403.20	K	1.90	NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C396645&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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