Benzene, 4-[(4-butylphenyl)ethynyl]-1,2-difluoro-

Other names: 4-n-butyl-3',4'-difluorodiphenylacetylene
Inchi: InChI=1S/C18H16F2/c1-2-3-4-14-5-7-15(8-6-14)9-10-16-11-12-17(19)18(20)13-16/h5-8,1
InchiKey: OAAKQGAJMFRMHO-UHFFFAOYSA-N
Formula: C18H16F2
SMILES: CCCCc1ccc(C#Cc2ccc(F)c(F)c2)cc1
Mol. weight [g/mol]: 270.32
CAS: 109970-65-2

Physical Properties

Property code	Value	Unit	Source
gf	109.79	kJ/mol	Joback Method
hf	-96.12	kJ/mol	Joback Method
hfus	38.57	kJ/mol	Joback Method
hvap	62.72	kJ/mol	Joback Method
log10ws	-6.19		Crippen Method
logp	4.707		Crippen Method
mcvol	211.900	ml/mol	McGowan Method
pc	1959.60	kPa	Joback Method
tb	687.08	K	Joback Method
tc	914.93	K	Joback Method
tf	490.30	K	Joback Method
vc	0.826	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	620.57	J/mol×K	876.96	Joback Method
cpg	548.56	J/mol×K	687.08	Joback Method
cpg	565.09	J/mol×K	725.06	Joback Method
cpg	580.50	J/mol×K	763.03	Joback Method
cpg	594.85	J/mol×K	801.01	Joback Method
cpg	608.19	J/mol×K	838.98	Joback Method
cpg	632.06	J/mol×K	914.93	Joback Method
hfust	25.30	kJ/mol	323.50	NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C109970652&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
hfust:	Enthalpy of fusion at a given temperature
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