1,4-BIS(ETHYNYL)BENZENE

Other names: 1,4-Bis(ethynyl)benzene
Benzene,1,4-diethynyl-
Inchi: InChI=1S/C10H6/c1-3-9-5-7-10(4-2)8-6-9/h1-2,5-8H
InchiKey: MVLGANVFCMOJHR-UHFFFAOYSA-N
Formula: C10H6
SMILES: C#Cc1ccc(C#C)cc1
Mol. weight [g/mol]: 126.16

Physical Properties

Property code	Value	Unit	Source
hf	452.27	kJ/mol	Cheméo Relay (1.0)
hfus	21.26	kJ/mol	Joback Method
ie	8.58 ± 0.02	eV	NIST Webbook
logp	1.649		Crippen Method
mcvol	110.800	ml/mol	McGowan Method
tb	472.57	K	Cheméo Relay (1.0)
tf	407.36	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	198.09	J/mol×K	440.10	Joback Method
cpg	209.35	J/mol×K	480.07	Joback Method
cpg	219.75	J/mol×K	520.03	Joback Method
cpg	229.36	J/mol×K	560.00	Joback Method
cpg	238.22	J/mol×K	599.96	Joback Method
cpg	246.40	J/mol×K	639.93	Joback Method
cpg	253.94	J/mol×K	679.89	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C935148&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point