BENZENE, 1-BROMO-4-ETHYNYL-

Inchi: InChI=1S/C8H5Br/c1-2-7-3-5-8(9)6-4-7/h1,3-6H
InchiKey: LTLVZQZDXQWLHU-UHFFFAOYSA-N
Formula: C8H5Br
SMILES: C#Cc1ccc(Br)cc1
Mol. weight [g/mol]: 181.03

Physical Properties

Property code	Value	Unit	Source
hf	318.42	kJ/mol	Cheméo Relay (1.0)
hfus	18.39	kJ/mol	Joback Method
ie	8.62	eV	NIST Webbook
log10ws	-3.60		Cheméo Relay (1.0)
logp	2.430		Crippen Method
mcvol	108.720	ml/mol	McGowan Method
tb	481.75	K	Cheméo Relay (1.0)
tf	345.49	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	182.23	J/mol×K	470.38	Joback Method
cpg	191.92	J/mol×K	511.80	Joback Method
cpg	200.81	J/mol×K	553.22	Joback Method
cpg	208.97	J/mol×K	594.63	Joback Method
cpg	216.44	J/mol×K	636.05	Joback Method
cpg	223.29	J/mol×K	677.47	Joback Method
cpg	229.58	J/mol×K	718.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source

tbrp	362.20	K	2.10	NIST Webbook

Sources

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
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=C766961&Units=SI

Legend

cpg:	Ideal gas heat capacity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tf:	Normal melting (fusion) point