Naphthalene, 1,8-di-1-propynyl-

Other names:	1,8-Bis(1-propynyl)naphthalene
	1,8-Di-1-propynylnaphthalene
Inchi:	InChI=1S/C16H12/c1-3-7-13-9-5-11-15-12-6-10-14(8-4-2)16(13)15/h5-6,9-12H,1-2H3
InchiKey:	GJRLHJRIHBWMNG-UHFFFAOYSA-N
Formula:	C16H12
SMILES:	CC#Cc1cccc2cccc(C#CC)c12
Mol. weight [g/mol]:	204.27
CAS:	22360-77-6

Physical Properties

Property code	Value	Unit	Source
gf	689.24	kJ/mol	Joback Method
hf	575.69	kJ/mol	Joback Method
hfus	33.72	kJ/mol	Joback Method
hvap	60.75	kJ/mol	Joback Method
ie	7.48	eV	NIST Webbook
log10ws	-5.51		Crippen Method
logp	3.583		Crippen Method
mcvol	175.880	ml/mol	McGowan Method
pc	2805.41	kPa	Joback Method
tb	639.10	K	Joback Method
tc	911.34	K	Joback Method
tf	566.44	K	Joback Method
vc	0.669	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	406.56	J/mol×K	639.10	Joback Method
cpg	422.73	J/mol×K	684.47	Joback Method
cpg	437.66	J/mol×K	729.85	Joback Method
cpg	451.47	J/mol×K	775.22	Joback Method
cpg	464.28	J/mol×K	820.59	Joback Method
cpg	476.19	J/mol×K	865.97	Joback Method

cpg	487.30	J/mol×K	911.34	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22360776&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

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