

1,5-(Ethano[1,4]benzeneoethano)naphthalene

Inchi:	InChI=1S/C20H18/c1-3-17-13-11-15-7-9-16(10-8-15)12-14-18-4-2-6-20(17)19(18)5-1/h1-
InchiKey:	PBFKBOVUUJKRHF-UHFFFAOYSA-N
Formula:	C20H18
SMILES:	<chem>c1cc2c3ccccc(c3c1)CCc1ccc(cc1)CC2</chem>
Mol. weight [g/mol]:	258.36
CAS:	60058-13-1

Physical Properties

Property code	Value	Unit	Source
gf	476.46	kJ/mol	Joback Method
hf	260.57	kJ/mol	Joback Method
hfus	26.45	kJ/mol	Joback Method
hvap	68.69	kJ/mol	Joback Method
ie	7.56	eV	NIST Webbook
log10ws	-6.36		Crippen Method
logp	4.724		Crippen Method
mvol	214.820	ml/mol	McGowan Method
pc	2293.71	kPa	Joback Method
tb	759.96	K	Joback Method
tc	1025.11	K	Joback Method
tf	456.92	K	Joback Method
vc	0.811	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	604.74	J/molxK	759.96	Joback Method
cpg	622.96	J/molxK	804.15	Joback Method
cpg	639.74	J/molxK	848.34	Joback Method
cpg	655.27	J/molxK	892.53	Joback Method
cpg	669.75	J/molxK	936.73	Joback Method
cpg	683.38	J/molxK	980.92	Joback Method
cpg	696.35	J/molxK	1025.11	Joback Method
dvisc	0.0014328	Paxs	456.92	Joback Method

dvisc	0.0009777	Paxs	507.43	Joback Method
dvisc	0.0007150	Paxs	557.93	Joback Method
dvisc	0.0005507	Paxs	608.44	Joback Method
dvisc	0.0004415	Paxs	658.95	Joback Method
dvisc	0.0003653	Paxs	709.45	Joback Method
dvisc	0.0003099	Paxs	759.96	Joback Method

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=C60058131&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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