

3,8-Methanocyclobuta[b]naphthalene,2a,3,8,8a-te

Inchi:	InChI=1S/C13H12/c1-2-4-9-8(3-1)12-7-13(9)11-6-5-10(11)12/h1-6,10-13H,7H2/t10-,11+,
InchiKey:	FLKOIGZBVYAFSE-FNFFVJSTSA-N
Formula:	C13H12
SMILES:	C1=CC2C3CC(c4ccccc43)C12
Mol. weight [g/mol]:	168.23
CAS:	54443-68-4

Physical Properties

Property code	Value	Unit	Source
gf	390.06	kJ/mol	Joback Method
hf	181.57	kJ/mol	Joback Method
hfus	23.98	kJ/mol	Joback Method
hvap	46.85	kJ/mol	Joback Method
ie	8.35 ± 0.05	eV	NIST Webbook
log10ws	-3.31		Crippen Method
logp	3.073		Crippen Method
mcvol	133.390	ml/mol	McGowan Method
pc	3062.55	kPa	Joback Method
tb	534.67	K	Joback Method
tc	766.93	K	Joback Method
tf	332.59	K	Joback Method
vc	0.527	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	333.26	J/mol×K	534.67	Joback Method
cpg	407.31	J/mol×K	728.22	Joback Method
cpg	394.89	J/mol×K	689.51	Joback Method
cpg	381.45	J/mol×K	650.80	Joback Method
cpg	366.81	J/mol×K	612.09	Joback Method
cpg	350.80	J/mol×K	573.38	Joback Method
cpg	418.85	J/mol×K	766.93	Joback Method
dvisc	0.0031612	Paxs	534.67	Joback Method

dvisc	0.0028584	Paxs	500.99	Joback Method
dvisc	0.0025472	Paxs	467.31	Joback Method
dvisc	0.0022297	Paxs	433.63	Joback Method
dvisc	0.0019085	Paxs	399.95	Joback Method
dvisc	0.0015875	Paxs	366.27	Joback Method
dvisc	0.0012721	Paxs	332.59	Joback Method

Sources

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=C54443684&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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