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	m3/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	Pa×s	534.67	Joback Method

dvisc	0.0028584	Pa×s	500.99	Joback Method
dvisc	0.0025472	Pa×s	467.31	Joback Method
dvisc	0.0022297	Pa×s	433.63	Joback Method
dvisc	0.0019085	Pa×s	399.95	Joback Method
dvisc	0.0015875	Pa×s	366.27	Joback Method
dvisc	0.0012721	Pa×s	332.59	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=C54443684&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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