[4.4.2]Propella-3,8,11-triene

Other names: 4a,8a-Ethenonaphthalene, 1,4,5,8-tetrahydro-
Inchi: InChI=1S/C12H14/c1-2-6-12-8-4-3-7-11(12,5-1)9-10-12/h1-4,9-10H,5-8H2
InchiKey: VGWHURSVJWSFCK-UHFFFAOYSA-N
Formula: C12H14
SMILES: C1=CCC23C=CC2(C1)CC=CC3
Mol. weight [g/mol]: 158.24
CAS: 20295-17-4

Physical Properties

Property code	Value	Unit	Source
gf	282.72	kJ/mol	Joback Method
hf	133.07	kJ/mol	Joback Method
hfus	4.94	kJ/mol	Joback Method
hvap	41.44	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
log10ws	-3.61		Crippen Method
logp	3.229		Crippen Method
mcvol	134.460	ml/mol	McGowan Method
pc	3568.53	kPa	Joback Method
tb	509.62	K	Joback Method
tc	762.15	K	Joback Method
tf	322.58	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	317.01	J/mol×K	509.62	Joback Method
cpg	336.61	J/mol×K	551.71	Joback Method
cpg	354.02	J/mol×K	593.80	Joback Method
cpg	369.69	J/mol×K	635.89	Joback Method
cpg	384.05	J/mol×K	677.98	Joback Method
cpg	397.54	J/mol×K	720.06	Joback Method
cpg	410.59	J/mol×K	762.15	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20295174&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