[4.2.2]Propella-2,4,7,9-tetraene

Inchi: InChI=1S/C10H8/c1-2-4-10-7-5-9(10,3-1)6-8-10/h1-8H
InchiKey: HLHKYPRYFGATQL-UHFFFAOYSA-N
Formula: C10H8
SMILES: C1=CC23C=CC2(C=C1)C=C3
Mol. weight [g/mol]: 128.17
CAS: 88090-34-0

Physical Properties

Property code	Value	Unit	Source
gf	320.04	kJ/mol	Joback Method
hf	244.45	kJ/mol	Joback Method
hfus	5.18	kJ/mol	Joback Method
hvap	36.94	kJ/mol	Joback Method
ie	8.06	eV	NIST Webbook
log10ws	-2.62		Crippen Method
logp	2.225		Crippen Method
mcvol	101.980	ml/mol	McGowan Method
pc	4468.24	kPa	Joback Method
tb	454.48	K	Joback Method
tc	699.27	K	Joback Method
tf	307.84	K	Joback Method
vc	0.400	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	213.76	J/mol×K	454.48	Joback Method
cpg	229.19	J/mol×K	495.28	Joback Method
cpg	242.31	J/mol×K	536.08	Joback Method
cpg	253.54	J/mol×K	576.88	Joback Method
cpg	263.28	J/mol×K	617.67	Joback Method
cpg	271.96	J/mol×K	658.47	Joback Method
cpg	279.99	J/mol×K	699.27	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C88090340&Units=SI

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