Tricyclo[4.3.1.0(1,6)]deca-2,4-diene

Inchi: InChI=1S/C10H12/c1-2-5-10-7-3-6-9(10,4-1)8-10/h1-2,4-5H,3,6-8H2
InchiKey: NBQVIMNMHQYULH-UHFFFAOYSA-N
Formula: C10H12
SMILES: C1=CC23CCCC2(C=C1)C3
Mol. weight [g/mol]: 132.20
CAS: 3463-81-8

Physical Properties

Property code	Value	Unit	Source
gf	260.12	kJ/mol	Joback Method
hf	190.00	kJ/mol	NIST Webbook
hfus	2.74	kJ/mol	Joback Method
hvap	36.36	kJ/mol	Joback Method
log10ws	-2.92		Crippen Method
logp	2.673		Crippen Method
mcvol	110.580	ml/mol	McGowan Method
pc	4067.32	kPa	Joback Method
tb	456.16	K	Joback Method
tc	695.62	K	Joback Method
tf	306.32	K	Joback Method
vc	0.427	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	243.89	J/mol×K	456.16	Joback Method
cpg	262.18	J/mol×K	496.07	Joback Method
cpg	278.15	J/mol×K	535.98	Joback Method
cpg	292.18	J/mol×K	575.89	Joback Method
cpg	304.66	J/mol×K	615.80	Joback Method
cpg	315.97	J/mol×K	655.71	Joback Method
cpg	326.50	J/mol×K	695.62	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=C3463818&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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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