

Tricyclo[4.4.2.0(1,6)dodeca-2,4,8-triene

Inchi: InChI=1S/C12H14/c1-2-6-12-8-4-3-7-11(12,5-1)9-10-12/h1-6H,7-10H2
InchiKey: ZBPOAKOSAXPANN-UHFFFAOYSA-N
Formula: C12H14
SMILES: C1=CC23CC=CCC2(C=C1)CC3
Mol. weight [g/mol]: 158.24
CAS: 60329-21-7

Physical Properties

Property code	Value	Unit	Source
gf	282.72	kJ/mol	Joback Method
hf	276.60	kJ/mol	NIST Webbook
hf	276.00	kJ/mol	NIST Webbook
hfus	4.94	kJ/mol	Joback Method
hvap	41.44	kJ/mol	Joback Method
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/molxK	509.62	Joback Method
cpg	336.61	J/molxK	551.71	Joback Method
cpg	354.02	J/molxK	593.80	Joback Method
cpg	369.69	J/molxK	635.89	Joback Method
cpg	384.05	J/molxK	677.98	Joback Method
cpg	397.54	J/molxK	720.06	Joback Method
cpg	410.59	J/molxK	762.15	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=C60329217&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
hvp:	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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