Tricyclo[4.4.2.0(1,6)dodeca-2,4,7,9-tetraene

Inchi: InChI=1S/C12H12/c1-2-6-12-8-4-3-7-11(12,5-1)9-10-12/h1-8H,9-10H2
InchiKey: GBIXITIROLAUBE-UHFFFAOYSA-N
Formula: C12H12
SMILES: C1=CC23C=CC=CC2(C=C1)CC3
Mol. weight [g/mol]: 156.22
CAS: 5181-34-0

Physical Properties

Property code	Value	Unit	Source
gf	312.68	kJ/mol	Joback Method
hf	378.30	kJ/mol	NIST Webbook
hfus	6.16	kJ/mol	Joback Method
hvap	41.74	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	3.005		Crippen Method
mcvol	130.160	ml/mol	McGowan Method
pc	3727.11	kPa	Joback Method
tb	508.78	K	Joback Method
tc	764.08	K	Joback Method
tf	323.34	K	Joback Method
vc	0.495	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.72	J/mol×K	508.78	Joback Method
cpg	317.92	J/mol×K	551.33	Joback Method
cpg	333.95	J/mol×K	593.88	Joback Method
cpg	348.26	J/mol×K	636.43	Joback Method
cpg	361.32	J/mol×K	678.98	Joback Method
cpg	373.57	J/mol×K	721.53	Joback Method
cpg	385.47	J/mol×K	764.08	Joback Method

Sources

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=C5181340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:
https://www.chemeo.com/cid/51-174-2/Tricyclo-4-4-2-0-1-6-dodeca-2-4-7-9-tetraene.pdf
Generated by Cheméo on 2024-05-01 06:42:29.470693529 +0000 UTC m=+16834998.391270844.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.