Tetraspiro[2.0.2.0.2.0.2.0]dodecane

Inchi: InChI=1S/C12H16/c1-2-9(1)10(3-4-10)12(7-8-12)11(9)5-6-11/h1-8H2
InchiKey: WDWKDXQBNGMXEI-UHFFFAOYSA-N
Formula: C12H16
SMILES: C1CC12C1(CC1)C1(CC1)C21CC1
Mol. weight [g/mol]: 160.26
CAS: 24375-17-5

Physical Properties

Property code	Value	Unit	Source
gf	375.96	kJ/mol	Joback Method
hf	172.77	kJ/mol	Joback Method
hfus	-2.45	kJ/mol	Joback Method
hvap	37.06	kJ/mol	Joback Method
ie	8.22	eV	NIST Webbook
log10ws	-3.35		Crippen Method
logp	3.121		Crippen Method
mcvol	125.640	ml/mol	McGowan Method
pc	3995.65	kPa	Joback Method
tb	500.48	K	Joback Method
tc	749.17	K	Joback Method
tf	425.10	K	Joback Method
vc	0.509	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.58	J/mol×K	500.48	Joback Method
cpg	359.25	J/mol×K	541.93	Joback Method
cpg	375.80	J/mol×K	583.38	Joback Method
cpg	390.08	J/mol×K	624.83	Joback Method
cpg	402.91	J/mol×K	666.28	Joback Method
cpg	415.12	J/mol×K	707.73	Joback Method
cpg	427.53	J/mol×K	749.17	Joback Method
hfust	21.00	kJ/mol	394.90	NIST Webbook

hsubt	74.90 ± 0.50	kJ/mol	318.00	NIST Webbook

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=C24375175&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
hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
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

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