Dispiro[2.0.2.1]heptane

Inchi: InChI=1S/C7H10/c1-2-6(1)5-7(6)3-4-7/h1-5H2
InchiKey: KGSOURBADOHWIS-UHFFFAOYSA-N
Formula: C7H10
SMILES: C1CC12CC21CC1
Mol. weight [g/mol]: 94.15
CAS: 33475-22-8

Physical Properties

Property code	Value	Unit	Source
chl	-4451.50 ± 3.50	kJ/mol	NIST Webbook
gf	211.24	kJ/mol	Joback Method
hf	302.80 ± 3.50	kJ/mol	NIST Webbook
hfl	267.80 ± 3.50	kJ/mol	NIST Webbook
hfus	-1.18	kJ/mol	Joback Method
hvap	35.10 ± 0.50	kJ/mol	NIST Webbook
hvap	35.00 ± 0.50	kJ/mol	NIST Webbook
hvap	35.00	kJ/mol	NIST Webbook
log10ws	-1.95		Crippen Method
logp	1.950		Crippen Method
mcvol	76.910	ml/mol	McGowan Method
pc	4910.80	kPa	Joback Method
tb	376.39	K	Joback Method
tc	590.93	K	Joback Method
tf	281.55	K	Joback Method
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	149.32	J/mol×K	376.39	Joback Method
cpg	166.61	J/mol×K	412.15	Joback Method
cpg	181.53	J/mol×K	447.90	Joback Method
cpg	194.37	J/mol×K	483.66	Joback Method
cpg	205.41	J/mol×K	519.42	Joback Method

cpg	214.95	J/mol×K	555.17	Joback Method
cpg	223.27	J/mol×K	590.93	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=C33475228&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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