Spiro[5.5]undecane-3-carboxylic acid

Inchi: InChI=1S/C12H20O2/c13-11(14)10-4-8-12(9-5-10)6-2-1-3-7-12/h10H,1-9H2,(H,13,14)
InchiKey: IMZALJRIJNIAON-UHFFFAOYSA-N
Formula: C12H20O2
SMILES: O=C(O)C1CCC2(CCCCC2)CC1
Mol. weight [g/mol]: 196.29
CAS: 18244-47-8

Physical Properties

Property code	Value	Unit	Source
gf	-160.07	kJ/mol	Joback Method
hf	-425.78	kJ/mol	Joback Method
hfus	12.00	kJ/mol	Joback Method
hvap	65.27	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.212		Crippen Method
mcvol	165.660	ml/mol	McGowan Method
pc	3138.51	kPa	Joback Method
tb	655.08	K	Joback Method
tc	876.82	K	Joback Method
tf	377.93	K	Joback Method
vc	0.605	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.09	J/mol×K	655.08	Joback Method
cpg	499.09	J/mol×K	692.04	Joback Method
cpg	516.03	J/mol×K	728.99	Joback Method
cpg	532.06	J/mol×K	765.95	Joback Method
cpg	547.32	J/mol×K	802.91	Joback Method
cpg	561.97	J/mol×K	839.86	Joback Method
cpg	576.14	J/mol×K	876.82	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=C18244478&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