9-(S)-Methyl-«delta»-5(10)-octalin-1,6-dione

Inchi: InChI=1S/C11H14O2/c1-11-6-5-9(12)7-8(11)3-2-4-10(11)13/h7H,2-6H2,1H3/t11-/m1/s1
InchiKey: DNHDRUMZDHWHKG-LLVKDONJSA-N
Formula: C11H14O2
SMILES: CC12CCC(=O)C=C1CCCC2=O
Mol. weight [g/mol]: 178.23
CAS: 33878-99-8

Physical Properties

Property code	Value	Unit	Source
gf	-107.79	kJ/mol	Joback Method
hf	-342.92	kJ/mol	Joback Method
hfus	4.60	kJ/mol	Joback Method
hvap	49.20	kJ/mol	Joback Method
log10ws	-2.39		Crippen Method
logp	2.035		Crippen Method
mcvol	142.970	ml/mol	McGowan Method
pc	3284.05	kPa	Joback Method
tb	626.33	K	Joback Method
tc	888.85	K	Joback Method
tf	413.39	K	Joback Method
vc	0.532	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	384.12	J/mol×K	626.33	Joback Method
cpg	402.84	J/mol×K	670.08	Joback Method
cpg	420.45	J/mol×K	713.84	Joback Method
cpg	437.09	J/mol×K	757.59	Joback Method
cpg	452.89	J/mol×K	801.35	Joback Method
cpg	468.00	J/mol×K	845.10	Joback Method
cpg	482.56	J/mol×K	888.85	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=C33878998&Units=SI

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