Lachnophyllum lactone

Inchi: InChI=1S/C10H8O2/c1-2-3-4-5-6-9-7-8-10(11)12-9/h2-3,6-8H,1H3/b3-2+,9-6-
InchiKey: ZNOFNADHELRFDF-KRIUCBPDSA-N
Formula: C10H8O2
SMILES: CC=CC#CC=C1C=CC(=O)O1
Mol. weight [g/mol]: 160.17

Physical Properties

Property code	Value	Unit	Source
gf	227.31	kJ/mol	Joback Method
hf	84.72	kJ/mol	Joback Method
hfus	26.88	kJ/mol	Joback Method
hvap	50.37	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	1.563		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
pc	3620.24	kPa	Joback Method
rinpol	1492.00		NIST Webbook
tb	561.88	K	Joback Method
tc	814.91	K	Joback Method
tf	424.53	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	275.21	J/mol×K	561.88	Joback Method
cpg	288.14	J/mol×K	604.05	Joback Method
cpg	300.23	J/mol×K	646.22	Joback Method
cpg	311.51	J/mol×K	688.39	Joback Method
cpg	322.02	J/mol×K	730.57	Joback Method
cpg	331.80	J/mol×K	772.74	Joback Method
cpg	340.89	J/mol×K	814.91	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=R409017&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume