4(Z),8(Z)-Matricaria lactone

Inchi: InChI=1S/C10H10O2/c1-2-3-4-5-6-9-7-8-10(11)12-9/h2-3,6H,7-8H2,1H3/b3-2-,9-6-
InchiKey: NUPAKTQITFGCSA-CITLEARMSA-N
Formula: C10H10O2
SMILES: CC=CC#CC=C1CCC(=O)O1
Mol. weight [g/mol]: 162.19

Physical Properties

Property code	Value	Unit	Source
gf	197.35	kJ/mol	Joback Method
hf	26.94	kJ/mol	Joback Method
hfus	25.66	kJ/mol	Joback Method
hvap	50.07	kJ/mol	Joback Method
log10ws	-2.76		Crippen Method
logp	1.787		Crippen Method
mcvol	131.140	ml/mol	McGowan Method
pc	3468.36	kPa	Joback Method
rinpol	1560.00		NIST Webbook
rinpol	1560.00		NIST Webbook
tb	562.72	K	Joback Method
tc	813.11	K	Joback Method
tf	423.77	K	Joback Method
vc	0.490	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	294.43	J/mol×K	562.72	Joback Method
cpg	308.76	J/mol×K	604.45	Joback Method
cpg	322.18	J/mol×K	646.18	Joback Method
cpg	334.75	J/mol×K	687.92	Joback Method
cpg	346.48	J/mol×K	729.65	Joback Method
cpg	357.42	J/mol×K	771.38	Joback Method
cpg	367.60	J/mol×K	813.11	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R634585&Units=SI
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

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