Perillic acid

Other names: 4-isopropenylcyclohex-1-enecarboxylic acid
Inchi: InChI=1S/C10H14O2/c1-7(2)8-3-5-9(6-4-8)10(11)12/h5,8H,1,3-4,6H2,2H3,(H,11,12)
InchiKey: CDSMSBUVCWHORP-UHFFFAOYSA-N
Formula: C10H14O2
SMILES: C=C(C)C1CC=C(C(=O)O)CC1
Mol. weight [g/mol]: 166.22
CAS: 7694-45-3

Physical Properties

Property code	Value	Unit	Source
gf	-108.35	kJ/mol	Joback Method
hf	-298.27	kJ/mol	Joback Method
hfus	17.42	kJ/mol	Joback Method
hvap	62.07	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.374		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	3265.31	kPa	Joback Method
rinpol	1467.00		NIST Webbook
rinpol	1500.00		NIST Webbook
rinpol	1467.00		NIST Webbook
tb	594.50	K	Joback Method
tc	798.35	K	Joback Method
tf	318.15	K	Joback Method
vc	0.521	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	350.00	J/mol×K	594.50	Joback Method
cpg	363.40	J/mol×K	628.48	Joback Method
cpg	376.02	J/mol×K	662.45	Joback Method
cpg	387.89	J/mol×K	696.43	Joback Method
cpg	399.02	J/mol×K	730.40	Joback Method

cpg	409.46	J/mol×K	764.38	Joback Method
cpg	419.23	J/mol×K	798.35	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=C7694453&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