Geranic acid

Other names: 2,6-Octadienoic acid, 3,7-dimethyl-
3,7-Dimethyl-2,6-octadienoic acid
3,7-dimethylocta-2,6-dienoic acid
Inchi: InChI=1S/C10H16O2/c1-8(2)5-4-6-9(3)7-10(11)12/h5,7H,4,6H2,1-3H3,(H,11,12)/b9-7+
InchiKey: ZHYZQXUYZJNEHD-VQHVLOKHSA-N
Formula: C10H16O2
SMILES: CC(C)=CCCC(C)=CC(=O)O
Mol. weight [g/mol]: 168.23
CAS: 459-80-3

Physical Properties

Property code	Value	Unit	Source
gf	-89.08	kJ/mol	Joback Method
hf	-299.68	kJ/mol	Joback Method
hfus	25.13	kJ/mol	Joback Method
hvap	61.36	kJ/mol	Joback Method
log10ws	-2.81		Crippen Method
logp	2.764		Crippen Method
mcvol	150.600	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1355.40		NIST Webbook
rinpol	1343.00		NIST Webbook
rinpol	1343.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2347.00		NIST Webbook
ripol	2356.00		NIST Webbook
tb	582.33	K	Joback Method
tc	767.56	K	Joback Method
tf	275.13	K	Joback Method
vc	0.583	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	362.94	J/mol×K	582.33	Joback Method
cpg	374.66	J/mol×K	613.20	Joback Method
cpg	385.77	J/mol×K	644.07	Joback Method
cpg	396.30	J/mol×K	674.94	Joback Method
cpg	406.28	J/mol×K	705.82	Joback Method
cpg	415.76	J/mol×K	736.69	Joback Method
cpg	424.77	J/mol×K	767.56	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C459803&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume