

Cyclopentanecarboxylic acid, 1-methyl-3-(1-methylethyl)-, cis-

Other names:	Cyclopentanecarboxylic acid, 3-isopropyl-1-methyl-, cis-Fencholic acid 1-Methyl-3-(1-methylethyl)-cyclopentanecarboxylic acid (fencholic acid)
Inchi:	InChI=1S/C10H18O2/c1-7(2)8-4-5-10(3,6-8)9(11)12/h7-8H,4-6H2,1-3H3,(H,11,12)
InchiKey:	IBDVYGIGYPWWBX-UHFFFAOYSA-N
Formula:	C10H16O2
SMILES:	CC(C)C1CCC(C)(C(=O)O)C1
Mol. weight [g/mol]:	168.23
CAS:	512-77-6

Physical Properties

Property code	Value	Unit	Source
gf	-211.51	kJ/mol	Joback Method
hf	-464.44	kJ/mol	Joback Method
hfus	12.53	kJ/mol	Joback Method
hvap	59.69	kJ/mol	Joback Method
log10ws	-2.28		Crippen Method
logp	2.533		Crippen Method
mcvol	148.340	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
tb	584.66	K	Joback Method
tc	783.28	K	Joback Method
tf	328.77	K	Joback Method
vc	0.552	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	445.36	J/molxK	717.08	Joback Method
cpg	457.43	J/molxK	750.18	Joback Method
cpg	390.87	J/molxK	584.66	Joback Method
cpg	405.61	J/molxK	617.76	Joback Method
cpg	419.54	J/molxK	650.87	Joback Method
cpg	432.76	J/molxK	683.97	Joback Method

cpg	469.06	J/mol×K	783.28	Joback Method
hvapt	91.60	kJ/mol	456.00	NIST Webbook
hvapt	77.50	kJ/mol	455.50	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C512776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvapt:	Enthalpy of vaporization at a given temperature
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

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