cis-DL-Pinonic acid

Inchi:	InChI=1S/C10H16O3/c1-6(11)8-4-7(5-9(12)13)10(8,2)3/h7-8H,4-5H2,1-3H3,(H,12,13)/t7-
InchiKey:	SIZDUQQDBXJXLQ-SFYZADRCSA-N
Formula:	C10H16O3
SMILES:	CC(=O)C1CC(CC(=O)O)C1(C)C
Mol. weight [g/mol]:	184.23
CAS:	17879-35-5

Physical Properties

Property code	Value	Unit	Source
chs	-5476.00	kJ/mol	NIST Webbook
gf	-333.60	kJ/mol	Joback Method
hf	-585.92	kJ/mol	Joback Method
hfs	-748.50	kJ/mol	NIST Webbook
hfus	20.82	kJ/mol	Joback Method
hvap	66.34	kJ/mol	Joback Method
log10ws	-1.56		Crippen Method
logp	1.712		Crippen Method
mcvol	149.910	ml/mol	McGowan Method
pc	2999.15	kPa	Joback Method
tb	630.03	K	Joback Method
tc	826.05	K	Joback Method
tf	392.98	K	Joback Method
vc	0.572	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.51	J/mol×K	630.03	Joback Method
cpg	422.36	J/mol×K	662.70	Joback Method
cpg	434.58	J/mol×K	695.37	Joback Method
cpg	446.27	J/mol×K	728.04	Joback Method
cpg	457.50	J/mol×K	760.71	Joback Method
cpg	468.37	J/mol×K	793.38	Joback Method
cpg	478.95	J/mol×K	826.05	Joback Method

Sources

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=C17879355&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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