

cis-1-Phenylcyclopropane-2-carboxylic acid

Inchi:	InChI=1S/C10H10O2/c11-10(12)9-6-8(9)7-4-2-1-3-5-7/h1-5,8-9H,6H2,(H,11,12)/t8-,9-/m0
InchiKey:	AHDDRJBFBDEPW-IUCAKERBSA-N
Formula:	C10H10O2
SMILES:	O=C(O)C1CC1c1ccccc1
Mol. weight [g/mol]:	162.19
CAS:	939-89-9

Physical Properties

Property code	Value	Unit	Source
chs	-5043.60 ± 2.40	kJ/mol	NIST Webbook
gf	-66.97	kJ/mol	Joback Method
hf	-225.55	kJ/mol	Joback Method
hfs	-320.00 ± 2.40	kJ/mol	NIST Webbook
hfus	20.59	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-1.83		Crippen Method
logp	1.875		Crippen Method
mcvol	124.580	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
tb	603.00	K	Joback Method
tc	817.06	K	Joback Method
tf	353.33	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	314.75	J/mol×K	603.00	Joback Method
cpg	326.83	J/mol×K	638.68	Joback Method
cpg	338.07	J/mol×K	674.35	Joback Method
cpg	348.51	J/mol×K	710.03	Joback Method
cpg	358.20	J/mol×K	745.71	Joback Method
cpg	367.22	J/mol×K	781.38	Joback Method
cpg	375.60	J/mol×K	817.06	Joback Method

dvisc	0.0046379	Pa×s	353.33	Joback Method
dvisc	0.0022088	Pa×s	394.94	Joback Method
dvisc	0.0012117	Pa×s	436.55	Joback Method
dvisc	0.0007380	Pa×s	478.17	Joback Method
dvisc	0.0004866	Pa×s	519.78	Joback Method
dvisc	0.0003413	Pa×s	561.39	Joback Method
dvisc	0.0002513	Pa×s	603.00	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C939899&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

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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