

Homocubane-4-carboxylic acid

Inchi:	InChI=1S/C10H10O2/c11-9(12)10-6-3-1-2-4(6)8(10)5(2)7(3)10/h2-8H,1H2,(H,11,12)
InchiKey:	MOOVPWJLDNIYBR-UHFFFAOYSA-N
Formula:	C10H10O2
SMILES:	O=C(O)C12C3C4CC5C3C1C5C42
Mol. weight [g/mol]:	162.19
CAS:	15844-05-0

Physical Properties

Property code	Value	Unit	Source
chs	-5285.00 ± 4.00	kJ/mol	NIST Webbook
gf	115.31	kJ/mol	Joback Method
hf	3.00	kJ/mol	NIST Webbook
hfs	-79.00 ± 4.00	kJ/mol	NIST Webbook
hfus	27.53	kJ/mol	Joback Method
hsub	82.00	kJ/mol	NIST Webbook
hsub	82.00	kJ/mol	NIST Webbook
hvap	57.73	kJ/mol	Joback Method
log10ws	-0.65		Crippen Method
logp	0.829		Crippen Method
mcvol	104.900	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
tb	568.56	K	Joback Method
tc	764.73	K	Joback Method
tf	435.21	K	Joback Method
vc	0.449	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	377.24	J/mol×K	732.04	Joback Method
cpg	329.09	J/mol×K	568.56	Joback Method
cpg	340.35	J/mol×K	601.26	Joback Method
cpg	350.58	J/mol×K	633.95	Joback Method
cpg	360.00	J/mol×K	666.65	Joback Method

cpg	368.82	J/mol×K	699.34	Joback Method
cpg	385.48	J/mol×K	764.73	Joback Method
cps	207.00	J/mol×K	298.00	NIST Webbook

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=C15844050&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
cps:	Solid phase 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
hsub:	Enthalpy of sublimation 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

Latest version available from:

<https://www.chemeo.com/cid/17-281-1/Homocubane-4-carboxylic-acid.pdf>

Generated by Cheméo on 2025-12-05 18:26:57.264285156 +0000 UTC m=+4707414.794325811.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.