

Isopiperitone

Inchi:	InChI=1S/C10H16O/c1-7(2)9-5-4-8(3)6-10(9)11/h6-7,9H,4-5H2,1-3H3
InchiKey:	YSTPAHQEHQSRJD-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CC(=O)C(C(C)C)CC1
Mol. weight [g/mol]:	152.23
CAS:	58615-39-7

Physical Properties

Property code	Value	Unit	Source
gf	-46.93	kJ/mol	Joback Method
hf	-292.08	kJ/mol	Joback Method
hfus	10.31	kJ/mol	Joback Method
hvap	43.10	kJ/mol	Joback Method
log10ws	-2.55		Crippen Method
logp	2.568		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2744.03	kPa	Joback Method
rinpol	1234.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1246.00		NIST Webbook
rinpol	1234.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1795.00		NIST Webbook
ripol	1838.00		NIST Webbook
ripol	1841.00		NIST Webbook
tb	519.27	K	Joback Method
tc	741.04	K	Joback Method
tf	276.34	K	Joback Method
vc	0.515	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
---------------	-------	------	-----------------	--------

cpg	321.40	J/mol×K	519.27	Joback Method
cpg	339.21	J/mol×K	556.23	Joback Method
cpg	356.17	J/mol×K	593.19	Joback Method
cpg	372.28	J/mol×K	630.16	Joback Method
cpg	387.53	J/mol×K	667.12	Joback Method
cpg	401.93	J/mol×K	704.08	Joback Method
cpg	415.47	J/mol×K	741.04	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=C58615397&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.cheméo.com/cid/70-270-4/Isopiperitone.pdf>

Generated by Cheméo on 2024-04-27 04:33:30.927093906 +0000 UTC m=+16481659.847671221.

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