

3-methyl-isochroman, 3e

Inchi:	InChI=1S/C10H12O/c1-8-6-9-4-2-3-5-10(9)7-11-8/h2-5,8H,6-7H2,1H3/t8-/m1/s1
InchiKey:	PYVOFBZTCULYKU-MRVPVSSYSA-N
Formula:	C10H12O
SMILES:	CC1Cc2ccccc2CO1
Mol. weight [g/mol]:	148.20

Physical Properties

Property code	Value	Unit	Source
gf	98.63	kJ/mol	Joback Method
hf	-90.03	kJ/mol	Joback Method
hfus	19.32	kJ/mol	Joback Method
hvap	45.39	kJ/mol	Joback Method
log10ws	-2.67		Crippen Method
logp	2.148		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1217.50		NIST Webbook
rinpol	1217.50		NIST Webbook
ripol	1736.00		NIST Webbook
tb	497.82	K	Joback Method
tc	728.25	K	Joback Method
tf	282.39	K	Joback Method
vc	0.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.13	J/molxK	497.82	Joback Method
cpg	342.99	J/molxK	689.85	Joback Method
cpg	330.78	J/molxK	651.44	Joback Method
cpg	317.65	J/molxK	613.04	Joback Method
cpg	303.54	J/molxK	574.63	Joback Method
cpg	288.38	J/molxK	536.23	Joback Method
cpg	354.33	J/molxK	728.25	Joback Method

dvisc	0.0003793	Paxs	497.82	Joback Method
dvisc	0.0004546	Paxs	461.91	Joback Method
dvisc	0.0005616	Paxs	426.01	Joback Method
dvisc	0.0007213	Paxs	390.11	Joback Method
dvisc	0.0009747	Paxs	354.20	Joback Method
dvisc	0.0014097	Paxs	318.29	Joback Method
dvisc	0.0022394	Paxs	282.39	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R256754&Units=SI

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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