1-methyl-isochroman, 1e'

Inchi: InChI=1S/C10H12O/c1-8-10-5-3-2-4-9(10)6-7-11-8/h2-5,8H,6-7H2,1H3/t8-/m0/s1
InchiKey: IRQLJDGOFUMMAW-QMMMGPOBSA-N
Formula: C10H12O
SMILES: CC1OCCc2ccccc21
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	-2.52		Crippen Method
logp	2.320		Crippen Method
mcvol	123.010	ml/mol	McGowan Method
pc	3395.98	kPa	Joback Method
rinpol	1220.00		NIST Webbook
rinpol	1220.00		NIST Webbook
ripol	1738.60		NIST Webbook
ripol	1738.60		NIST Webbook
tb	497.82	K	Joback Method
tc	728.25	K	Joback Method
tf	282.39	K	Joback Method
vc	0.458	m3/kmol	Joback Method

Temperature Dependent Properties

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

cpg	354.33	J/mol×K	728.25	Joback Method
dvisc	0.0003793	Pa×s	497.82	Joback Method
dvisc	0.0004546	Pa×s	461.91	Joback Method
dvisc	0.0005616	Pa×s	426.01	Joback Method
dvisc	0.0007213	Pa×s	390.11	Joback Method
dvisc	0.0009747	Pa×s	354.20	Joback Method
dvisc	0.0014097	Pa×s	318.29	Joback Method
dvisc	0.0022394	Pa×s	282.39	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R256729&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