

Isocyclocitral 2

Inchi:	InChI=1S/C10H16O/c1-7-4-8(2)10(6-11)9(3)5-7/h4,6,8-10H,5H2,1-3H3
InchiKey:	YJSUCBQWLKRPDL-UHFFFAOYSA-N
Formula:	C10H16O
SMILES:	CC1=CC(C)C(C=O)C(C)C1
Mol. weight [g/mol]:	152.23

Physical Properties

Property code	Value	Unit	Source
gf	-36.84	kJ/mol	Joback Method
hf	-275.36	kJ/mol	Joback Method
hfus	18.75	kJ/mol	Joback Method
hvap	45.34	kJ/mol	Joback Method
log10ws	-2.31		Crippen Method
logp	2.424		Crippen Method
mcvol	138.170	ml/mol	McGowan Method
pc	2646.11	kPa	Joback Method
rinpol	1141.80		NIST Webbook
ripol	1549.00		NIST Webbook
ripol	1549.00		NIST Webbook
tb	491.21	K	Joback Method
tc	695.98	K	Joback Method
tf	256.64	K	Joback Method
vc	0.529	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	313.91	J/mol×K	491.21	Joback Method
cpg	391.54	J/mol×K	661.85	Joback Method
cpg	377.58	J/mol×K	627.72	Joback Method
cpg	362.84	J/mol×K	593.59	Joback Method
cpg	347.33	J/mol×K	559.47	Joback Method
cpg	331.02	J/mol×K	525.34	Joback Method
cpg	404.74	J/mol×K	695.98	Joback Method

dvisc	0.0003370	Paxs	491.21	Joback Method
dvisc	0.0003967	Paxs	452.12	Joback Method
dvisc	0.0004817	Paxs	413.02	Joback Method
dvisc	0.0006090	Paxs	373.92	Joback Method
dvisc	0.0008133	Paxs	334.83	Joback Method
dvisc	0.0011726	Paxs	295.74	Joback Method
dvisc	0.0018898	Paxs	256.64	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=R499728&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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