Dolichodial

Inchi: InChI=1S/C10H14O2/c1-7-3-4-9(8(2)5-11)10(7)6-12/h5-7,9-10H,2-4H2,1H3/t7-,9?,10?/m
InchiKey: BORBLDJNKYHVJP-WFRXLMHJSA-N
Formula: C10H14O2
SMILES: C=C(C=O)C1CCC(C)C1C=O
Mol. weight [g/mol]: 166.22

Physical Properties

Property code	Value	Unit	Source
gf	-65.30	kJ/mol	Joback Method
hf	-285.45	kJ/mol	Joback Method
hfus	19.72	kJ/mol	Joback Method
hvap	50.34	kJ/mol	Joback Method
log10ws	-1.59		Crippen Method
logp	1.603		Crippen Method
mcvol	139.740	ml/mol	McGowan Method
pc	2862.74	kPa	Joback Method
rinpol	1164.00		NIST Webbook
rinpol	1164.00		NIST Webbook
tb	528.02	K	Joback Method
tc	734.55	K	Joback Method
tf	273.16	K	Joback Method
vc	0.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.76	J/mol×K	528.02	Joback Method
cpg	351.54	J/mol×K	562.44	Joback Method
cpg	366.44	J/mol×K	596.86	Joback Method
cpg	380.49	J/mol×K	631.28	Joback Method
cpg	393.72	J/mol×K	665.70	Joback Method
cpg	406.15	J/mol×K	700.13	Joback Method
cpg	417.81	J/mol×K	734.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R345176&Units=SI
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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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