(-)-Car-3-en-2-one

Inchi: InChI=1S/C10H14O/c1-6-4-5-7-8(9(6)11)10(7,2)3/h4,7-8H,5H2,1-3H3
InchiKey: SAFIHMIEMQFPDA-UHFFFAOYSA-N
Formula: C10H14O
SMILES: CC1=CCC2C(C1=O)C2(C)C
Mol. weight [g/mol]: 150.22
CAS: 53585-45-8

Physical Properties

Property code	Value	Unit	Source
gf	27.26	kJ/mol	Joback Method
hf	-206.78	kJ/mol	Joback Method
hfus	10.94	kJ/mol	Joback Method
hvap	41.59	kJ/mol	Joback Method
log10ws	-2.21		Crippen Method
logp	2.178		Crippen Method
mcvol	127.310	ml/mol	McGowan Method
pc	3002.44	kPa	Joback Method
rinpol	1300.00		NIST Webbook
rinpol	1254.30		NIST Webbook
rinpol	1254.30		NIST Webbook
ripol	1881.00		NIST Webbook
tb	513.48	K	Joback Method
tc	740.08	K	Joback Method
tf	335.98	K	Joback Method
vc	0.491	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	307.39	J/mol×K	513.48	Joback Method
cpg	324.08	J/mol×K	551.25	Joback Method
cpg	339.67	J/mol×K	589.01	Joback Method
cpg	354.29	J/mol×K	626.78	Joback Method
cpg	368.08	J/mol×K	664.55	Joback Method

cpg	381.17	J/mol×K	702.31	Joback Method
cpg	393.70	J/mol×K	740.08	Joback Method

Sources

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=C53585458&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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