trans-2,6-Dimethyl-heptan-5-olide

Inchi: InChI=1S/C9H16O2/c1-6(2)4-8-5-7(3)9(10)11-8/h6-8H,4-5H2,1-3H3/t7-,8-/m1/s1
InchiKey: SYDVLDZWCVEHRQ-HTQZYQBOSA-N
Formula: C9H16O2
SMILES: CC(C)CC1CC(C)C(=O)O1
Mol. weight [g/mol]: 156.22

Physical Properties

Property code	Value	Unit	Source
gf	-157.41	kJ/mol	Joback Method
hf	-463.93	kJ/mol	Joback Method
hfus	18.04	kJ/mol	Joback Method
hvap	43.95	kJ/mol	Joback Method
log10ws	-1.98		Crippen Method
logp	1.984		Crippen Method
mcvol	134.250	ml/mol	McGowan Method
pc	2767.17	kPa	Joback Method
ripol	1856.00		NIST Webbook
ripol	1856.00		NIST Webbook
tb	510.26	K	Joback Method
tc	722.36	K	Joback Method
tf	277.64	K	Joback Method
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	324.05	J/mol×K	510.26	Joback Method
cpg	341.28	J/mol×K	545.61	Joback Method
cpg	357.73	J/mol×K	580.96	Joback Method
cpg	373.41	J/mol×K	616.31	Joback Method
cpg	388.31	J/mol×K	651.66	Joback Method
cpg	402.43	J/mol×K	687.01	Joback Method
cpg	415.77	J/mol×K	722.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R326328&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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