Salsolene ketone

Inchi: InChI=1S/C15H24O/c1-10(2)14-6-5-12-9-13(14)8-11(3)4-7-15(12)16/h8,10,12-14H,4-7,9
InchiKey: MGLWWZNRAQRXLJ-CTOLLULRSA-N
Formula: C15H24O
SMILES: CC1=CC2CC(CCC2C(C)C)C(=O)CC1
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	24.01	kJ/mol	Joback Method
hf	-355.14	kJ/mol	Joback Method
hfus	18.27	kJ/mol	Joback Method
hvap	54.17	kJ/mol	Joback Method
log10ws	-4.06		Crippen Method
logp	3.984		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
rinpol	1803.00		NIST Webbook
tb	644.28	K	Joback Method
tc	876.76	K	Joback Method
tf	339.35	K	Joback Method
vc	0.736	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	569.07	J/mol×K	644.28	Joback Method
cpg	593.12	J/mol×K	683.03	Joback Method
cpg	615.62	J/mol×K	721.77	Joback Method
cpg	636.59	J/mol×K	760.52	Joback Method
cpg	656.06	J/mol×K	799.27	Joback Method
cpg	674.05	J/mol×K	838.02	Joback Method
cpg	690.56	J/mol×K	876.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R233855&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume