7-Oxabicyclo[4.1.0]heptan-2-one, 4,4,6-trimethyl-

Other names: Isophorone epoxide
Isophorone oxide
2,3-Epoxy-3,5,5-trimethylcyclohexanone
2,3-Epoxy-3,5,5-trimethyl-1-cyclohexanone
Inchi: InChI=1S/C9H14O2/c1-8(2)4-6(10)7-9(3,5-8)11-7/h7H,4-5H2,1-3H3
InchiKey: ROTNQFPVXVZSRL-UHFFFAOYSA-N
Formula: C9H14O2
SMILES: CC1(C)CC(=O)C2OC2(C)C1
Mol. weight [g/mol]: 154.21
CAS: 10276-21-8

Physical Properties

Property code	Value	Unit	Source
gf	-93.10	kJ/mol	Joback Method
hf	-349.21	kJ/mol	Joback Method
hfus	9.20	kJ/mol	Joback Method
hvap	41.77	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.533		Crippen Method
mcvol	123.390	ml/mol	McGowan Method
pc	3403.91	kPa	Joback Method
rinpol	1333.00		NIST Webbook
rinpol	1333.00		NIST Webbook
tb	513.65	K	Joback Method
tc	748.55	K	Joback Method
tf	361.90	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	309.41	J/mol×K	513.65	Joback Method
cpg	326.04	J/mol×K	552.80	Joback Method
cpg	341.34	J/mol×K	591.95	Joback Method

cpg	355.57	J/mol×K	631.10	Joback Method
cpg	368.98	J/mol×K	670.25	Joback Method
cpg	381.84	J/mol×K	709.40	Joback Method
cpg	394.39	J/mol×K	748.55	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C10276218&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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