(E)-«alpha»-Atlantone

Other names: «alpha»-(E)-Atlantone
trans-«alpha»-Atlantone
Inchi: InChI=1S/C15H22O/c1-11(2)9-15(16)10-13(4)14-7-5-12(3)6-8-14/h5,9-10,14H,6-8H2,1-4
InchiKey: OJEFBZMKKJTKKK-JWAFFJSPSA-N
Formula: C15H22O
SMILES: CC(C)=CC(=O)C=C(C)C1CC=C(C)CC1
Mol. weight [g/mol]: 218.33
CAS: 108645-54-1

Physical Properties

Property code	Value	Unit	Source
gf	134.62	kJ/mol	Joback Method
hf	-150.02	kJ/mol	Joback Method
hfus	26.66	kJ/mol	Joback Method
hvap	57.19	kJ/mol	Joback Method
log10ws	-4.60		Crippen Method
logp	4.214		Crippen Method
mcvol	200.020	ml/mol	McGowan Method
pc	1966.56	kPa	Joback Method
rinpol	1779.00		NIST Webbook
rinpol	1781.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1744.00		NIST Webbook
rinpol	1785.10		NIST Webbook
tb	628.24	K	Joback Method
tc	847.12	K	Joback Method
tf	291.32	K	Joback Method
vc	0.762	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.72	J/mol×K	628.24	Joback Method
cpg	541.09	J/mol×K	664.72	Joback Method
cpg	559.24	J/mol×K	701.20	Joback Method
cpg	576.24	J/mol×K	737.68	Joback Method
cpg	592.18	J/mol×K	774.16	Joback Method
cpg	607.10	J/mol×K	810.64	Joback Method
cpg	621.10	J/mol×K	847.12	Joback Method

Sources

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=C108645541&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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