14-Oxy-«alpha»-muurolene

Other names: 14-Oxi-«alpha»-muurolene
14-Oxy-2-muurolene
Inchi: InChI=1S/C15H22O/c1-10(2)13-7-5-12(9-16)14-6-4-11(3)8-15(13)14/h5,8-10,13-15H,4,6
InchiKey: DNHAZRYDTSOZHV-UHFFFAOYSA-N
Formula: C15H22O
SMILES: CC1=CC2C(CC1)C(C=O)=CCC2C(C)C
Mol. weight [g/mol]: 218.33
CAS: 69394-04-3

Physical Properties

Property code	Value	Unit	Source
gf	79.51	kJ/mol	Joback Method
hf	-250.55	kJ/mol	Joback Method
hfus	23.98	kJ/mol	Joback Method
hvap	57.43	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2053.03	kPa	Joback Method
rinpol	1776.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1765.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1810.00		NIST Webbook
ripol	2227.00		NIST Webbook
tb	624.99	K	Joback Method
tc	842.80	K	Joback Method
tf	329.93	K	Joback Method
vc	0.740	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	531.53	J/mol×K	624.99	Joback Method
cpg	552.07	J/mol×K	661.29	Joback Method
cpg	571.34	J/mol×K	697.59	Joback Method
cpg	589.38	J/mol×K	733.89	Joback Method
cpg	606.26	J/mol×K	770.20	Joback Method
cpg	622.01	J/mol×K	806.50	Joback Method
cpg	636.68	J/mol×K	842.80	Joback Method
dvisc	0.0025245	Pa×s	329.93	Joback Method
dvisc	0.0015545	Pa×s	379.11	Joback Method
dvisc	0.0010699	Pa×s	428.28	Joback Method
dvisc	0.0007953	Pa×s	477.46	Joback Method
dvisc	0.0006249	Pa×s	526.64	Joback Method
dvisc	0.0005116	Pa×s	575.81	Joback Method
dvisc	0.0004322	Pa×s	624.99	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=C69394043&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
dvisc: Dynamic viscosity
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