Khusimone

Inchi: InChI=1S/C14H20O/c1-9-11-4-5-12(15)14(11)7-6-10(8-14)13(9,2)3/h10-11H,1,4-8H2,2-3
InchiKey: BDHSOIIDXCBNPA-PEMBBPQUSA-N
Formula: C14H20O
SMILES: C=C1C2CCC(=O)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 204.31

Physical Properties

Property code	Value	Unit	Source
gf	136.85	kJ/mol	Joback Method
hf	-169.53	kJ/mol	Joback Method
hfus	9.05	kJ/mol	Joback Method
hvap	48.64	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.348		Crippen Method
mcvol	172.810	ml/mol	McGowan Method
pc	2472.73	kPa	Joback Method
rinpol	1604.00		NIST Webbook
rinpol	1606.00		NIST Webbook
rinpol	1584.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1577.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1603.00		NIST Webbook
rinpol	1578.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1616.00		NIST Webbook
rinpol	1592.00		NIST Webbook
rinpol	1604.00		NIST Webbook
ripol	2175.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2190.00		NIST Webbook
ripol	2175.00		NIST Webbook
tb	611.27	K	Joback Method
tc	853.73	K	Joback Method
tf	419.78	K	Joback Method
vc	0.660	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	487.80	J/mol×K	611.27	Joback Method
cpg	508.81	J/mol×K	651.68	Joback Method
cpg	528.58	J/mol×K	692.09	Joback Method
cpg	547.44	J/mol×K	732.50	Joback Method
cpg	565.72	J/mol×K	772.91	Joback Method
cpg	583.74	J/mol×K	813.32	Joback Method
cpg	601.83	J/mol×K	853.73	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R198386&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume