occidol

Inchi: InChI=1S/C15H22O/c1-10-5-6-11(2)14-9-12(15(3,4)16)7-8-13(10)14/h5-6,12,16H,7-9H2,
InchiKey: AFBBWQXTLZVDEE-UHFFFAOYSA-N
Formula: C15H22O
SMILES: Cc1ccc(C)c2c1CCC(C(C)(C)O)C2
Mol. weight [g/mol]: 218.33
CAS: 5986-36-7

Physical Properties

Property code	Value	Unit	Source
gf	73.61	kJ/mol	Joback Method
hf	-245.15	kJ/mol	Joback Method
hfus	20.19	kJ/mol	Joback Method
hvap	68.71	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.179		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2254.67	kPa	Joback Method
rinpol	1822.00		NIST Webbook
rinpol	1824.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1822.00		NIST Webbook
rinpol	1832.00		NIST Webbook
rinpol	1844.00		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1860.00		NIST Webbook
ripol	2658.00		NIST Webbook
ripol	2653.00		NIST Webbook
tb	684.18	K	Joback Method
tc	895.36	K	Joback Method
tf	400.45	K	Joback Method
vc	0.725	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	550.13	J/mol×K	684.18	Joback Method
cpg	623.08	J/mol×K	860.17	Joback Method
cpg	610.27	J/mol×K	824.97	Joback Method
cpg	596.65	J/mol×K	789.77	Joback Method
cpg	582.13	J/mol×K	754.57	Joback Method
cpg	566.64	J/mol×K	719.38	Joback Method
cpg	635.13	J/mol×K	895.36	Joback Method
dvisc	0.0000694	Pa×s	684.18	Joback Method
dvisc	0.0000988	Pa×s	636.89	Joback Method
dvisc	0.0001490	Pa×s	589.60	Joback Method
dvisc	0.0002413	Pa×s	542.32	Joback Method
dvisc	0.0004285	Pa×s	495.03	Joback Method
dvisc	0.0008591	Pa×s	447.74	Joback Method
dvisc	0.0020299	Pa×s	400.45	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=C5986367&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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