

C22H34O

Inchi:	InChI=1S/C22H34O/c23-22(19-10-13-1-4-16(19)7-13,20-11-14-2-5-17(20)8-14)21-12-15
InchiKey:	JNDULIEHFWRQA-UHFFFAOYSA-N
Formula:	C22H34O
SMILES:	OC(C1CC2CCC1C2)(C1CC2CCC1C2)C1CC2CCC1C2
Mol. weight [g/mol]:	314.50
CAS:	17687-75-1

Physical Properties

Property code	Value	Unit	Source
gf	305.45	kJ/mol	Joback Method
hf	-301.09	kJ/mol	Joback Method
hfus	35.13	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.60		Crippen Method
logp	5.026		Crippen Method
mcvol	261.550	ml/mol	McGowan Method
pc	1648.43	kPa	Joback Method
tb	830.95	K	Joback Method
tc	1055.50	K	Joback Method
tf	485.30	K	Joback Method
vc	0.991	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	981.25	J/mol×K	830.95	Joback Method
cpg	1004.47	J/mol×K	868.38	Joback Method
cpg	1026.49	J/mol×K	905.80	Joback Method
cpg	1047.56	J/mol×K	943.23	Joback Method
cpg	1067.90	J/mol×K	980.65	Joback Method
cpg	1087.75	J/mol×K	1018.08	Joback Method
cpg	1107.36	J/mol×K	1055.50	Joback Method
dvisc	0.0156000	Pa×s	485.30	Joback Method
dvisc	0.0121474	Pa×s	542.91	Joback Method

dvisc	0.0099240	Pa×s	600.52	Joback Method
dvisc	0.0083996	Pa×s	658.12	Joback Method
dvisc	0.0073029	Pa×s	715.73	Joback Method
dvisc	0.0064831	Pa×s	773.34	Joback Method
dvisc	0.0058511	Pa×s	830.95	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C17687751&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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