

Norketoagarofuran

Inchi:	InChI=1S/C14H22O2/c1-12(2)10-6-8-13(3)7-4-5-11(15)14(13,9-10)16-12/h10H,4-9H2,1-3
InchiKey:	GZGANJGCMJYOEK-ZLKJLUDKSA-N
Formula:	C14H22O2
SMILES:	CC1(C)OC23CC1CCC2(C)CCCC3=O
Mol. weight [g/mol]:	222.32

Physical Properties

Property code	Value	Unit	Source
gf	-19.94	kJ/mol	Joback Method
hf	-376.69	kJ/mol	Joback Method
hfus	9.79	kJ/mol	Joback Method
hvap	52.01	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	3.093		Crippen Method
mcvol	182.980	ml/mol	McGowan Method
pc	2579.34	kPa	Joback Method
rinpola	1556.00		NIST Webbook
rinpola	1555.00		NIST Webbook
rinpola	1555.00		NIST Webbook
rinpola	1556.00		NIST Webbook
tb	643.57	K	Joback Method
tc	898.60	K	Joback Method
tf	453.05	K	Joback Method
vc	0.688	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.02	J/molxK	643.57	Joback Method
cpg	565.23	J/molxK	686.08	Joback Method
cpg	586.50	J/molxK	728.58	Joback Method
cpg	607.32	J/molxK	771.09	Joback Method
cpg	628.21	J/molxK	813.59	Joback Method
cpg	649.68	J/molxK	856.10	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=R613048&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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

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