«alpha»-agorofuran

Other names: «alpha»-Agarofuran
Inchi: InChI=1S/C15H24O/c1-11-6-5-8-14(4)9-7-12-10-15(11,14)16-13(12,2)3/h6,12H,5,7-10H2
InchiKey: ZLQADKTVJQXDIG-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1=CCCC2(C)CCC3CC12OC3(C)C
Mol. weight [g/mol]: 220.35
CAS: 5956-12-7

Physical Properties

Property code	Value	Unit	Source
gf	131.40	kJ/mol	Joback Method
hf	-213.32	kJ/mol	Joback Method
hfus	13.70	kJ/mol	Joback Method
hvap	50.94	kJ/mol	Joback Method
log10ws	-4.47		Crippen Method
logp	4.080		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2313.61	kPa	Joback Method
rinpol	1539.00		NIST Webbook
rinpol	1556.10		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1581.00		NIST Webbook
rinpol	1555.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1536.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1569.00		NIST Webbook
rinpol	1539.00		NIST Webbook
rinpol	1545.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	1535.00		NIST Webbook
rinpol	1552.00		NIST Webbook

rinpol	1543.00		NIST Webbook
rinpol	1567.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1878.00		NIST Webbook
ripol	1861.00		NIST Webbook
ripol	1907.00		NIST Webbook
tb	602.77	K	Joback Method
tc	842.98	K	Joback Method
tf	409.38	K	Joback Method
vc	0.723	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.54	J/mol×K	602.77	Joback Method
cpg	559.70	J/mol×K	642.81	Joback Method
cpg	580.49	J/mol×K	682.84	Joback Method
cpg	600.39	J/mol×K	722.88	Joback Method
cpg	619.85	J/mol×K	762.91	Joback Method
cpg	639.36	J/mol×K	802.95	Joback Method
cpg	659.36	J/mol×K	842.98	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=C5956127&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
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