3a,4,5,7a-tetrahydro-3,6-dimethyl-2(3H)-benzofuranone

Other names: tetrahydro-3,6-dimethyl-2(3H)-benzofuranone, 3a,4,5,7a
2(3H)-Benzofuranone, 3a,4,5,7a-tetrahydro-3,6-dimethyl-
3,6-dimethyl-3a,4,5,7a-tetrahydro-3H-1-benzofuran-2-one

Inchi: InChI=1S/C10H14O2/c1-6-3-4-8-7(2)10(11)12-9(8)5-6/h5,7-9H,3-4H2,1-2H3

InchiKey: NQWBFQXRASPNLB-UHFFFAOYSA-N

Formula: C10H14O2

SMILES: CC1=CC2OC(=O)C(C)C2CC1

Mol. weight [g/mol]: 166.22

CAS: 57743-63-2

Physical Properties

Property code	Value	Unit	Source
gf	-77.57	kJ/mol	Joback Method
hf	-366.34	kJ/mol	Joback Method
hfus	21.02	kJ/mol	Joback Method
hvap	47.60	kJ/mol	Joback Method
log10ws	-2.14		Crippen Method
logp	1.904		Crippen Method
mcvol	133.180	ml/mol	McGowan Method
pc	2989.32	kPa	Joback Method
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
rinpol	1456.00		NIST Webbook
ripol	2220.00		NIST Webbook
ripol	2220.00		NIST Webbook
ripol	2220.00		NIST Webbook
ripol	2188.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2188.00		NIST Webbook
tb	548.73	K	Joback Method
tc	780.29	K	Joback Method
tf	331.61	K	Joback Method
vc	0.498	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	339.65	J/mol×K	548.73	Joback Method
cpg	357.85	J/mol×K	587.32	Joback Method
cpg	375.01	J/mol×K	625.92	Joback Method
cpg	391.16	J/mol×K	664.51	Joback Method
cpg	406.31	J/mol×K	703.10	Joback Method
cpg	420.46	J/mol×K	741.70	Joback Method
cpg	433.65	J/mol×K	780.29	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C57743632&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
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