Isobornyl formate

Other names:	Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, formate, exo- 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl formate, exo- Isoborneol, formate Bicyclo(2.2.1)heptan-2-ol, 1,7,7-trimethyl-, 2-formate, (1R,2R,4R)-rel- exo-1,7,7-trimethylbicyclo[2.2.1]hept-2-yl formate
Inchi:	InChI=1S/C11H18O2/c1-10(2)8-4-5-11(10,3)9(6-8)13-7-12/h7-9H,4-6H2,1-3H3
InchiKey:	RDWUNORUTVEHJF-UHFFFAOYSA-N
Formula:	C11H18O2
SMILES:	CC1(C)C2CCC1(C)C(OC=O)C2
Mol. weight [g/mol]:	182.26
CAS:	1200-67-5

Physical Properties

Property code	Value	Unit	Source
gf	-79.78	kJ/mol	Joback Method
hf	-358.93	kJ/mol	Joback Method
hfus	11.44	kJ/mol	Joback Method
hvap	46.29	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	2.374		Crippen Method
mcvol	151.570	ml/mol	McGowan Method
pc	2746.90	kPa	Joback Method
rinpol	1236.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1231.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1245.00		NIST Webbook
rinpol	1237.00		NIST Webbook
rinpol	1235.00		NIST Webbook
rinpol	1206.00		NIST Webbook

rinpol	1228.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1206.00		NIST Webbook
rinpol	1240.00		NIST Webbook
rinpol	1233.00		NIST Webbook
rinpol	1244.00		NIST Webbook
rinpol	1227.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1229.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1596.00		NIST Webbook
ripol	1574.00		NIST Webbook
ripol	1596.00		NIST Webbook
tb	531.05	K	Joback Method
tc	745.15	K	Joback Method
tf	349.64	K	Joback Method
vc	0.587	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.47	J/mol×K	531.05	Joback Method
cpg	407.28	J/mol×K	566.73	Joback Method
cpg	423.82	J/mol×K	602.42	Joback Method
cpg	439.31	J/mol×K	638.10	Joback Method
cpg	453.97	J/mol×K	673.79	Joback Method
cpg	468.00	J/mol×K	709.47	Joback Method
cpg	481.62	J/mol×K	745.15	Joback Method
hvapt	53.50	kJ/mol	412.00	NIST Webbook

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=C1200675&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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