

Bicyclo[2.2.1]heptan-2-ol, 1,7,7-trimethyl-, formate, endo-

Other names:	Borneol, formate Bornyl formate 1,7,7-Trimethylbicyclo[2.2.1]hept-2-yl formate, endo- Endoisobornylformate endo-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/t8?,9-,11
InchiKey:	RDWUNORUTVEHJF-YUCVTWSNSA-N
Formula:	C11H18O2
SMILES:	CC1(C)C2CCC1(C)C(OC=O)C2
Mol. weight [g/mol]:	182.26
CAS:	7492-41-3

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	1228.00		NIST Webbook
rinpol	1223.00		NIST Webbook
rinpol	1236.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1239.00		NIST Webbook
rinpol	1199.00		NIST Webbook
rinpol	1217.00		NIST Webbook
rinpol	1208.00		NIST Webbook
rinpol	1232.00		NIST Webbook
rinpol	1228.00		NIST Webbook
rinpol	1208.00		NIST Webbook
ripol	1592.00		NIST Webbook

ripol	1610.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1543.00		NIST Webbook
ripol	1597.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1610.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
ripol	1588.00		NIST Webbook
tb	531.05	K	Joback Method
tc	745.15	K	Joback Method
tf	349.64	K	Joback Method
vc	0.587	m ³ /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	52.70	kJ/mol	403.50	NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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=C7492413&Units=SI>

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

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