3-Oxatricyclo[4.1.1.0(2,4)]octane, 2,7,7-trimethyl-

Other names: 2,7,7-Trimethyl-3-oxatricyclo[4.1.1.02,4]octane
Pinane, 2,3-epoxy-
«alpha»-Pinene epoxide
«alpha»-Pinene oxide
2,3-Epoxypinane
«alpha»-Pinene 2,3-oxide
«alpha»-Pinene epoxide (Isomer 1)
«alpha»-Pinene epoxide (Isomer 2)
«alpha»-Pinene oxyde
3-Oxatricyclo[4.1.1.02,4]octane, 2,7,7-trimethyl-

Inchi: InChI=1S/C10H16O/c1-9(2)6-4-7(9)10(3)8(5-6)11-10/h6-8H,4-5H2,1-3H3

InchiKey: NQFUSWIGRKFAHK-UHFFFAOYSA-N

Formula: C10H16O

SMILES: CC1(C)C2CC3OC3(C)C1C2

Mol. weight [g/mol]: 152.23

CAS: 1686-14-2

Physical Properties

Property code	Value	Unit	Source
gf	115.15	kJ/mol	Joback Method
hf	-167.37	kJ/mol	Joback Method
hfus	15.69	kJ/mol	Joback Method
hvap	53.60	kJ/mol	NIST Webbook
log10ws	-2.28		Crippen Method
logp	2.210		Crippen Method
mcvol	125.050	ml/mol	McGowan Method
pc	3093.29	kPa	Joback Method
rinpol	1100.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1100.00		NIST Webbook
rinpol	1087.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1095.00		NIST Webbook
rinpol	1099.00		NIST Webbook
rinpol	1110.00		NIST Webbook
rinpol	1099.00		NIST Webbook

rinpol	1097.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1071.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1096.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1106.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1085.00	NIST Webbook
rinpol	1082.00	NIST Webbook
rinpol	1060.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1086.00	NIST Webbook
rinpol	1090.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1095.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1100.00	NIST Webbook
rinpol	1099.00	NIST Webbook
rinpol	1105.00	NIST Webbook
rinpol	1094.00	NIST Webbook
rinpol	1091.00	NIST Webbook
rinpol	1065.00	NIST Webbook
rinpol	1103.00	NIST Webbook
rinpol	1100.00	NIST Webbook
ripol	1384.00	NIST Webbook
ripol	1384.00	NIST Webbook

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ripol	1384.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1353.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1384.00		NIST Webbook
ripol	1384.00		NIST Webbook
tb	462.24	K	Joback Method
tc	676.49	K	Joback Method
tf	325.69	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	308.28	J/mol×K	462.24	Joback Method
cpg	327.25	J/mol×K	497.95	Joback Method
cpg	344.37	J/mol×K	533.66	Joback Method
cpg	359.91	J/mol×K	569.37	Joback Method
cpg	374.13	J/mol×K	605.08	Joback Method
cpg	387.30	J/mol×K	640.78	Joback Method
cpg	399.67	J/mol×K	676.49	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	375.70	K	6.70	NIST Webbook

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=C1686142&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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume