

(1«alpha»,3«alpha»,5«alpha»,7«alpha»)-3,8,8-trimethyl-4-oxatricyclo[5.1.0.0(3,5)]octane

Other names:	4-Oxatricyclo[5.1.0.0(3,5)]octane, 3,8,8-trimethyl-, (1«alpha»,3«alpha»,5«alpha»,7«alpha»)-
Inchi:	CC12CC3(C)C(C)(C)C3(C)CC1O2
InchiKey:	ZDZDFGKYHPOEMW-KLHWPWHYSA-N
Formula:	C10H16O
SMILES:	CC12CC3(C)C(C)(C)C3(C)CC1O2
Mol. weight [g/mol]:	152.23
CAS:	35671-18-2

Physical Properties

Property code	Value	Unit	Source
chl	-6073.70 ± 1.60	kJ/mol	NIST Webbook
chl	-6073.70 ± 1.60	kJ/mol	NIST Webbook
gf	121.01	kJ/mol	Joback Method
hf	-98.00 ± 3.00	kJ/mol	NIST Webbook
hf	-98.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-148.10 ± 1.70	kJ/mol	NIST Webbook
hfl	-148.10 ± 1.70	kJ/mol	NIST Webbook
hfus	8.27	kJ/mol	Joback Method
hvap	50.10	kJ/mol	NIST Webbook
hvap	50.00 ± 2.00	kJ/mol	NIST Webbook
hvap	50.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-3.12		Crippen Method
logp	2.990		Crippen Method
mcvol	153.230	ml/mol	McGowan Method
pc	2770.08	kPa	Joback Method
tb	508.48	K	Joback Method
tc	734.74	K	Joback Method
tf	396.03	K	Joback Method
vc	0.598	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.10	J/mol×K	508.48	Joback Method

cpg	421.61	J/mol×K	546.19	Joback Method
cpg	439.01	J/mol×K	583.90	Joback Method
cpg	454.80	J/mol×K	621.61	Joback Method
cpg	469.51	J/mol×K	659.32	Joback Method
cpg	483.63	J/mol×K	697.03	Joback Method
cpg	497.69	J/mol×K	734.74	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=C35671182&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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