(1«alpha»,3«beta»,5«beta»,7«alpha»)-3,8,8-trimeth

Other names: 4-Oxatricyclo[5.1.0.0(3,5)-]octane, 3,8,8-trimethyl-, (1«alpha»,3«beta»,5«beta»,7«alpha»)-
Inchi: InChI=1S/C12H20O/c1-9(2)11(4)6-8-10(3,13-8)7-12(9,11)5/h8H,6-7H2,1-5H3/t8-,10+,11-
InchiKey: ZDZDFGKYHPOEMW-GMNPVEAJSA-N
Formula: C10H16O
SMILES: CC12CC3(C)C(C)(C)C3(C)CC1O2
Mol. weight [g/mol]: 152.23
CAS: 21218-11-1

Physical Properties

Property code	Value	Unit	Source
chl	-6065.40 ± 1.50	kJ/mol	NIST Webbook
chl	-6065.40 ± 1.50	kJ/mol	NIST Webbook
gf	121.01	kJ/mol	Joback Method
hf	-107.00 ± 3.00	kJ/mol	NIST Webbook
hf	-107.00 ± 3.00	kJ/mol	NIST Webbook
hfl	-156.40 ± 1.50	kJ/mol	NIST Webbook
hfl	-156.40 ± 1.50	kJ/mol	NIST Webbook
hfus	8.27	kJ/mol	Joback Method
hvap	49.00 ± 2.00	kJ/mol	NIST Webbook
hvap	49.00 ± 2.00	kJ/mol	NIST Webbook
hvap	49.40	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	m3/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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C21218111&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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