Edulan II

Other names:	2H-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-, (2S-cis)- 2,5,5,8a-Tetramethyl-3,5,6,8a-tetrahydro-2H-chromene-, (2S-cis)- cis-Edulan
Inchi:	InChI=1S/C13H20O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h5,7,9-10H,6,8H2,1-4H3/t1
InchiKey:	HUXGOQHTDHIKSS-ZWNOBZJWSA-N
Formula:	C13H20O
SMILES:	CC1CC=C2C(C)(C)CC=CC2(C)O1
Mol. weight [g/mol]:	192.30
CAS:	41678-30-2

Physical Properties

Property code	Value	Unit	Source
gf	77.16	kJ/mol	Joback Method
hf	-208.46	kJ/mol	Joback Method
hfus	15.81	kJ/mol	Joback Method
hvap	48.19	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.466		Crippen Method
mcvol	169.580	ml/mol	McGowan Method
pc	2497.50	kPa	Joback Method
rinpol	1328.00		NIST Webbook
rinpol	1247.00		NIST Webbook
tb	553.46	K	Joback Method
tc	786.87	K	Joback Method
tf	342.24	K	Joback Method
vc	0.633	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	432.15	J/mol×K	553.46	Joback Method
cpg	452.71	J/mol×K	592.36	Joback Method
cpg	471.81	J/mol×K	631.26	Joback Method
cpg	489.73	J/mol×K	670.16	Joback Method

cpg	506.72	J/mol×K	709.06	Joback Method
cpg	523.07	J/mol×K	747.97	Joback Method
cpg	539.04	J/mol×K	786.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C41678302&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

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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