2H-1-Benzopyran, 3,5,6,8a-tetrahydro-2,5,5,8a-tetramethyl-, trans-

Other names: Edulan I
trans-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-MFKMUULPSA-N
Formula: C13H20O
SMILES: CC1CC=C2C(C)(C)CC=CC2(C)O1
Mol. weight [g/mol]: 192.30
CAS: 41678-29-9

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	1313.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1309.00		NIST Webbook
rinpol	1315.00		NIST Webbook
rinpol	1326.00		NIST Webbook
rinpol	1314.00		NIST Webbook
rinpol	1321.00		NIST Webbook
ripol	1620.00		NIST Webbook
ripol	1602.00		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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41678299&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

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