2H-1-Benzopyran, 3,4,4a,5,6,8a-hexahydro-2,5,5,8a-tetramethyl-, (2«alpha»,4a«alpha»,8a«alpha»)-

Other names: (2«alpha»,4a«alpha»,8a«alpha»)-3,4,4a,5,6,8a-Hexahydro-2,5,5,8a-tetramethyl-2H-1-ben
Dihydroedulan II
Edulan II dihydro
Dihydroedulan II (cis)

Inchi: InChI=1S/C13H22O/c1-10-6-7-11-12(2,3)8-5-9-13(11,4)14-10/h5,9-11H,6-8H2,1-4H3

InchiKey: IVTQSEFLDHBCDZ-UHFFFAOYSA-N

Formula: C13H22O

SMILES: CC1CCC2C(C)(C)CC=CC2(C)O1

Mol. weight [g/mol]: 194.31

CAS: 41678-32-4

Physical Properties

Property code	Value	Unit	Source
gf	49.12	kJ/mol	Joback Method
hf	-275.11	kJ/mol	Joback Method
hfus	16.04	kJ/mol	Joback Method
hvap	46.93	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	3.546		Crippen Method
mcvol	173.880	ml/mol	McGowan Method
pc	2367.97	kPa	Joback Method
rinpol	1296.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
rinpol	1318.00		NIST Webbook
ripol	1569.00		NIST Webbook
ripol	1569.00		NIST Webbook
tb	544.65	K	Joback Method
tc	774.56	K	Joback Method
tf	324.72	K	Joback Method
vc	0.646	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	451.15	J/mol×K	544.65	Joback Method
cpg	473.87	J/mol×K	582.97	Joback Method
cpg	494.99	J/mol×K	621.29	Joback Method
cpg	514.78	J/mol×K	659.61	Joback Method
cpg	533.50	J/mol×K	697.93	Joback Method
cpg	551.39	J/mol×K	736.24	Joback Method
cpg	568.71	J/mol×K	774.56	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41678324&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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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