(3S,3aR,6R,8aS)-7,7-Dimethyl-8-methyleneoctahyd acid

Other names: 1H-3a,6-Methanoazulene-3-carboxylic acid, octahydro-7,7-dimethyl-8-methylene-, (3S,3aR,6R,8aS)-
1H-3a,6-Methanoazulene-3-carboxylic acid, octahydro-7,7-dimethyl-8-methylene-, [3S-(3«alpha»,3a«alpha»,6«alpha»,8a«alpha»)]-
1H-3a«alpha»,6-Methanoazulene-3-carboxylic acid, 2,3«beta»,4,5,6«beta»,7,8,8a«alpha»-octahydro-7,7-dimethyl-8-methylene-
Khusenic acid
Vetivenic acid
Zizanoic acid
(+)-Zizanoic acid

Inchi: [3S-(3«alpha»,3a«alpha»,6«alpha»,8a«alpha»)]-octahydro-7,7-dimethyl-8-methylene-1H-
InChI=1S/C15H22O2/c1-9-11-4-5-12(13(16)17)15(11)7-6-10(8-15)14(9,2)3/h10-12H,1,4-
InchiKey: IJGMVUXEZUEDJR-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: C=C1C2CCC(C(=O)O)C23CCC(C3)C1(C)C
Mol. weight [g/mol]: 234.33
CAS: 16203-25-1

Physical Properties

Property code	Value	Unit	Source
gf	-5.59	kJ/mol	Joback Method
hf	-337.62	kJ/mol	Joback Method
hfus	18.89	kJ/mol	Joback Method
hvap	69.73	kJ/mol	Joback Method
log10ws	-3.53		Crippen Method
logp	3.480		Crippen Method
mcvol	192.770	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook
rinpol	1860.00		NIST Webbook
rinpol	1803.00		NIST Webbook
rinpol	1823.00		NIST Webbook
rinpol	1812.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1811.00		NIST Webbook
tb	707.71	K	Joback Method
tc	921.86	K	Joback Method
tf	469.34	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.02	J/mol×K	707.71	Joback Method
cpg	613.45	J/mol×K	743.40	Joback Method
cpg	630.39	J/mol×K	779.09	Joback Method
cpg	647.10	J/mol×K	814.78	Joback Method
cpg	663.83	J/mol×K	850.48	Joback Method
cpg	680.83	J/mol×K	886.17	Joback Method
cpg	698.35	J/mol×K	921.86	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C16203251&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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