1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, acetate, [3R-(3«alpha»,3a«beta»,6«alpha»,7«beta»,8a«alph

Other names: 8«beta»H-Cedran-8-ol, acetate
Cedryl acetate
Acetic acid, cedrol ester
Cedranyl acetate
1H-3a,7-Methanoazulen-6-ol, octahydro-3,6,8,8-tetramethyl-, acetate

Inchi: [3R-(3«alpha»,3a«beta»,6«alpha»,7«beta»,8a«alpha»)]-octahydro-3,6,8,8-tetramethyl-1H-
InChI=1S/C17H28O2/c1-11-6-7-13-15(3,4)14-10-17(11,13)9-8-16(14,5)19-12(2)18/h11,1
acetate
InchiKey: HQKQRXZEXPXXIG-IUGWZREUSA-N
Formula: C17H28O2
SMILES: CC(=O)OC1(C)CCC23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 264.40
CAS: 77-54-3

Physical Properties

Property code	Value	Unit	Source
gf	-23.21	kJ/mol	Joback Method
hf	-448.23	kJ/mol	Joback Method
hfus	17.10	kJ/mol	Joback Method
hvap	58.30	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	4.181		Crippen Method
mcvol	225.250	ml/mol	McGowan Method
pc	1845.16	kPa	Joback Method
rinpol	1759.00		NIST Webbook
rinpol	1766.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1768.00		NIST Webbook
rinpol	1768.30		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1758.00		NIST Webbook
rinpol	1779.70		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1763.00		NIST Webbook
rinpol	1771.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1759.00		NIST Webbook

rinpol	1762.00		NIST Webbook
ripol	2147.00		NIST Webbook
ripol	2143.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2173.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2150.00		NIST Webbook
tb	680.12	K	Joback Method
tc	906.53	K	Joback Method
tf	459.27	K	Joback Method
vc	0.858	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	690.49	J/mol×K	680.12	Joback Method
cpg	713.37	J/mol×K	717.86	Joback Method
cpg	735.56	J/mol×K	755.59	Joback Method
cpg	757.45	J/mol×K	793.33	Joback Method
cpg	779.41	J/mol×K	831.06	Joback Method
cpg	801.82	J/mol×K	868.80	Joback Method
cpg	825.06	J/mol×K	906.53	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C77543&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