Neointermedeol

Inchi: InChI=1S/C15H28O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h11-13,16H,5-10H2
InchiKey: PWTWAHBPEXYEQQ-MLGYPOCJSA-N
Formula: C15H26O
SMILES: CC(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]: 222.37
CAS: 5945-72-2

Physical Properties

Property code	Value	Unit	Source
gf	-17.14	kJ/mol	Joback Method
hf	-399.68	kJ/mol	Joback Method
hfus	12.59	kJ/mol	Joback Method
hvap	62.87	kJ/mol	Joback Method
log10ws	-4.30		Crippen Method
logp	4.000		Crippen Method
mcvol	206.360	ml/mol	McGowan Method
pc	2115.83	kPa	Joback Method
rinpol	1662.00		NIST Webbook
rinpol	1661.00		NIST Webbook
rinpol	1602.00		NIST Webbook
rinpol	1656.00		NIST Webbook
rinpol	1641.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1601.00		NIST Webbook
rinpol	1597.00		NIST Webbook
rinpol	1600.00		NIST Webbook
rinpol	1662.10		NIST Webbook
rinpol	1669.70		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1660.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1600.00		NIST Webbook
ripol	2139.00		NIST Webbook
ripol	2093.00		NIST Webbook
ripol	2138.00		NIST Webbook
ripol	2148.00		NIST Webbook
tb	656.04	K	Joback Method

tc	865.65	K	Joback Method
tf	365.75	K	Joback Method
vc	0.764	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	617.08	J/mol×K	656.04	Joback Method
cpg	638.19	J/mol×K	690.98	Joback Method
cpg	658.35	J/mol×K	725.91	Joback Method
cpg	677.78	J/mol×K	760.85	Joback Method
cpg	696.66	J/mol×K	795.78	Joback Method
cpg	715.22	J/mol×K	830.72	Joback Method
cpg	733.64	J/mol×K	865.65	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=C5945722&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

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