

Intermedeol

Inchi:	InChI=1S/C15H26O/c1-11(2)12-6-9-14(3)7-5-8-15(4,16)13(14)10-12/h12-13,16H,1,5-10H
InchiKey:	DPQYOKVMVCQHMY-LRMVUMKSA-N
Formula:	C15H26O
SMILES:	C=C(C)C1CCC2(C)CCCC(C)(O)C2C1
Mol. weight [g/mol]:	222.37
CAS:	6168-59-8

Physical Properties

Property code	Value	Unit	Source
gf	64.59	kJ/mol	Joback Method
hf	-278.76	kJ/mol	Joback Method
hfus	13.52	kJ/mol	Joback Method
hvap	62.67	kJ/mol	Joback Method
log10ws	-4.39		Crippen Method
logp	3.920		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinpol	1666.50		NIST Webbook
rinpol	1674.60		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1666.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1645.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1663.00		NIST Webbook
rinpol	1665.00		NIST Webbook
rinpol	1627.00		NIST Webbook
rinpol	1629.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1626.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1651.00		NIST Webbook

ripol	1677.00		NIST Webbook
ripol	1667.00		NIST Webbook
ripol	2262.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2247.00		NIST Webbook
ripol	2218.00		NIST Webbook
ripol	2264.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2264.00		NIST Webbook
tb	653.04	K	Joback Method
tc	865.92	K	Joback Method
tf	365.03	K	Joback Method
vc	0.752	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.33	J/mol×K	653.04	Joback Method
cpg	613.82	J/mol×K	688.52	Joback Method
cpg	633.38	J/mol×K	724.00	Joback Method
cpg	652.21	J/mol×K	759.48	Joback Method
cpg	670.53	J/mol×K	794.96	Joback Method
cpg	688.57	J/mol×K	830.44	Joback Method
cpg	706.54	J/mol×K	865.92	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=C6168598&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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
rinpolar:	Non-polar retention indices
ripolar:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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