

Drimenol

Inchi: InChI=1S/C15H26O/c1-11-6-7-13-14(2,3)8-5-9-15(13,4)12(11)10-16/h6,12-13,16H,5,7-10H
InchiKey: HMWSKUKBAWWOJL-UHFFFAOYSA-N
Formula: C15H26O
SMILES: CC1=CCC2C(C)(C)CCCC2(C)C1CO
Mol. weight [g/mol]: 222.37
CAS: 468-68-8

Physical Properties

Property code	Value	Unit	Source
gf	5.63	kJ/mol	Joback Method
hf	-348.09	kJ/mol	Joback Method
hfus	16.94	kJ/mol	Joback Method
hvap	64.21	kJ/mol	Joback Method
log10ws	-4.04		Crippen Method
logp	3.778		Crippen Method
mcvol	202.060	ml/mol	McGowan Method
pc	2141.36	kPa	Joback Method
rinpol	1749.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1788.10		NIST Webbook
rinpol	1794.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1759.00		NIST Webbook
rinpol	1777.10		NIST Webbook
rinpol	1770.00		NIST Webbook
rinpol	1745.00		NIST Webbook
rinpol	1757.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1750.00		NIST Webbook
rinpol	1761.00		NIST Webbook
rinpol	1750.00		NIST Webbook

ripol	2494.00		NIST Webbook
ripol	2525.00		NIST Webbook
tb	660.62	K	Joback Method
tc	868.94	K	Joback Method
tf	394.03	K	Joback Method
vc	0.756	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	593.85	J/mol×K	660.62	Joback Method
cpg	613.42	J/mol×K	695.34	Joback Method
cpg	632.18	J/mol×K	730.06	Joback Method
cpg	650.33	J/mol×K	764.78	Joback Method
cpg	668.06	J/mol×K	799.50	Joback Method
cpg	685.56	J/mol×K	834.22	Joback Method
cpg	703.03	J/mol×K	868.94	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=C468688&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
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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