

Prezizaan-15-ol

Inchi:	InChI=1S/C15H26O/c1-10-4-5-13-14(2,3)12(9-16)11-6-7-15(10,13)8-11/h10-13,16H,4-9H
InchiKey:	KTMJGGMQCFLMFK-VJYADGHSA-N
Formula:	C15H26O
SMILES:	CC1CCC2C(C)(C)C(CO)C3CCC12C3
Mol. weight [g/mol]:	222.37

Physical Properties

Property code	Value	Unit	Source
gf	62.54	kJ/mol	Joback Method
hf	-329.62	kJ/mol	Joback Method
hfus	19.52	kJ/mol	Joback Method
hvap	62.52	kJ/mol	Joback Method
log10ws	-3.60		Crippen Method
logp	3.467		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2193.84	kPa	Joback Method
rinsol	1745.00		NIST Webbook
tb	650.01	K	Joback Method
tc	856.17	K	Joback Method
tf	401.49	K	Joback Method
vc	0.743	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.04	J/mol×K	650.01	Joback Method
cpg	619.09	J/mol×K	684.37	Joback Method
cpg	638.22	J/mol×K	718.73	Joback Method
cpg	656.66	J/mol×K	753.09	Joback Method
cpg	674.65	J/mol×K	787.45	Joback Method
cpg	692.39	J/mol×K	821.81	Joback Method
cpg	710.12	J/mol×K	856.17	Joback Method

Sources

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=R397954&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Latest version available from:

<https://www.chemeo.com/cid/61-052-6/Prezizaan-15-ol.pdf>

Generated by Cheméo on 2024-04-19 20:07:23.617287484 +0000 UTC m=+15846492.537864796.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.