

«beta»-davan-2-ol

Inchi:	InChI=1S/C15H24O3/c1-6-15(5)10-8-13(18-15)11(2)12(16)7-9-14(3,4)17/h6-7,9,11,13,17
InchiKey:	WQUKMIHCFQFPQG-AJPPRRINSA-N
Formula:	C15H24O3
SMILES:	C=CC1(C)CCC(C(C)C(=O)C=CC(C)(C)O)O1
Mol. weight [g/mol]:	252.35

Physical Properties

Property code	Value	Unit	Source
gf	-84.63	kJ/mol	Joback Method
hf	-465.74	kJ/mol	Joback Method
hfus	24.96	kJ/mol	Joback Method
hvap	73.32	kJ/mol	Joback Method
log10ws	-3.43		Crippen Method
logp	2.642		Crippen Method
mcvol	216.060	ml/mol	McGowan Method
pc	2068.00	kPa	Joback Method
rinpol	1725.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1713.00		NIST Webbook
rinpol	1668.00		NIST Webbook
rinpol	1717.00		NIST Webbook
rinpol	1725.00		NIST Webbook
tb	723.62	K	Joback Method
tc	929.03	K	Joback Method
tf	407.27	K	Joback Method
vc	0.803	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	641.58	J/molxK	723.62	Joback Method
cpg	657.78	J/molxK	757.86	Joback Method
cpg	673.27	J/molxK	792.09	Joback Method
cpg	688.20	J/molxK	826.33	Joback Method

cpg	702.71	J/mol×K	860.56	Joback Method
cpg	716.96	J/mol×K	894.80	Joback Method
cpg	731.08	J/mol×K	929.03	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=R303583&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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