Davanaether I

Inchi: InChI=1S/C15H26O2/c1-6-15(5)10-8-13(17-15)11(2)12-7-9-14(3,4)16-12/h6,11-13H,1,7-
InchiKey: MWVSMYWOHUWFCW-UHFFFAOYSA-N
Formula: C15H26O2
SMILES: C=CC1(C)CCC(C(C)C2CCC(C)(C)O2)O1
Mol. weight [g/mol]: 238.37

Physical Properties

Property code	Value	Unit	Source
gf	35.28	kJ/mol	Joback Method
hf	-386.02	kJ/mol	Joback Method
hfus	23.18	kJ/mol	Joback Method
hvap	54.54	kJ/mol	Joback Method
log10ws	-4.12		Crippen Method
logp	3.704		Crippen Method
mcvol	207.930	ml/mol	McGowan Method
pc	1989.43	kPa	Joback Method
ripol	1914.00		NIST Webbook
ripol	1914.00		NIST Webbook
tb	614.44	K	Joback Method
tc	840.66	K	Joback Method
tf	356.31	K	Joback Method
vc	0.768	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	590.98	J/mol×K	614.44	Joback Method
cpg	614.19	J/mol×K	652.14	Joback Method
cpg	636.07	J/mol×K	689.85	Joback Method
cpg	656.90	J/mol×K	727.55	Joback Method
cpg	676.91	J/mol×K	765.26	Joback Method
cpg	696.36	J/mol×K	802.96	Joback Method
cpg	715.51	J/mol×K	840.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R328502&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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