Clovenol

Inchi: InChI=1S/C15H26O/c1-13(2)8-9-15-7-5-12(16)14(3,10-15)6-4-11(13)15/h11-12,16H,4-10
InchiKey: ZCECGQRKYOENSP-FXYBZAJKSA-N
Formula: C15H26O
SMILES: CC1(C)CCC23CCC(O)C(C)(CCC12)C3
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	52.66	kJ/mol	Joback Method
hf	-300.20	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	61.85	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	3.754		Crippen Method
mcvol	195.500	ml/mol	McGowan Method
pc	2421.88	kPa	Joback Method
rinpol	1581.00		NIST Webbook
rinpol	1581.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2222.00		NIST Webbook
ripol	2238.00		NIST Webbook
tb	659.19	K	Joback Method
tc	879.30	K	Joback Method
tf	426.11	K	Joback Method
vc	0.734	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	596.54	J/mol×K	659.19	Joback Method
cpg	617.00	J/mol×K	695.88	Joback Method
cpg	636.71	J/mol×K	732.56	Joback Method
cpg	656.04	J/mol×K	769.25	Joback Method
cpg	675.35	J/mol×K	805.93	Joback Method

cpg	694.99	J/mol×K	842.62	Joback Method
cpg	715.33	J/mol×K	879.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R423419&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
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