Elema-1,3-dien-7-ol

Inchi: InChI=1S/C15H26O/c1-7-14(6)8-9-15(16,12(4)5)10-13(14)11(2)3/h7,12-13,16H,1-2,8-10
InchiKey: IEPFBZDLASGILR-QLFBSQMISA-N
Formula: C15H26O
SMILES: C=CC1(C)CCC(O)(C(C)C)CC1C(=C)C
Mol. weight [g/mol]: 222.37

Physical Properties

Property code	Value	Unit	Source
gf	101.34	kJ/mol	Joback Method
hf	-225.25	kJ/mol	Joback Method
hfus	12.68	kJ/mol	Joback Method
hvap	61.52	kJ/mol	Joback Method
log10ws	-4.35		Crippen Method
logp	3.942		Crippen Method
mcvol	208.620	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinpol	1531.00		NIST Webbook
tb	638.27	K	Joback Method
tc	839.54	K	Joback Method
tf	333.85	K	Joback Method
vc	0.778	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	582.51	J/mol×K	638.27	Joback Method
cpg	601.35	J/mol×K	671.82	Joback Method
cpg	619.36	J/mol×K	705.36	Joback Method
cpg	636.70	J/mol×K	738.91	Joback Method
cpg	653.55	J/mol×K	772.45	Joback Method
cpg	670.08	J/mol×K	806.00	Joback Method
cpg	686.46	J/mol×K	839.54	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=R281646&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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