Diepicedrene-1-oxide

Inchi: InChI=1S/C15H24O/c1-8-5-6-11-14(3,4)10-7-15(8,11)13-12(16-13)9(10)2/h8-13H,5-7H2,
InchiKey: HETWPUJFGKDFMN-UHFFFAOYSA-N
Formula: C15H24O
SMILES: CC1C2OC2C23CC1C(C)(C)C2CCC3C
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	190.48	kJ/mol	Joback Method
hf	-244.61	kJ/mol	Joback Method
hfus	26.81	kJ/mol	Joback Method
hvap	49.61	kJ/mol	Joback Method
log10ws	-3.54		Crippen Method
logp	3.482		Crippen Method
mcvol	184.640	ml/mol	McGowan Method
pc	2086.93	kPa	Joback Method
rinpol	1551.00		NIST Webbook
tb	578.31	K	Joback Method
tc	798.81	K	Joback Method
tf	387.98	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.31	J/mol×K	578.31	Joback Method
cpg	566.49	J/mol×K	615.06	Joback Method
cpg	588.09	J/mol×K	651.81	Joback Method
cpg	608.41	J/mol×K	688.56	Joback Method
cpg	627.78	J/mol×K	725.31	Joback Method
cpg	646.49	J/mol×K	762.06	Joback Method
cpg	664.85	J/mol×K	798.81	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U156110&Units=SI

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