«alpha»-Copaen-8«alpha»-ol

Inchi: InChI=1S/C15H24O/c1-8(2)10-7-12(16)15(4)11-6-5-9(3)14(15)13(10)11/h5,8,10-14,16H,
InchiKey: CLFNFYDETASPQF-QNAZDQAQSA-N
Formula: C15H24O
SMILES: CC1=CCC2C3C(C(C)C)CC(O)C2(C)C13
Mol. weight [g/mol]: 220.35

Physical Properties

Property code	Value	Unit	Source
gf	98.02	kJ/mol	Joback Method
hf	-297.67	kJ/mol	Joback Method
hfus	25.22	kJ/mol	Joback Method
hvap	64.06	kJ/mol	Joback Method
log10ws	-3.56		Crippen Method
logp	3.242		Crippen Method
mcvol	191.200	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1555.00		NIST Webbook
rinpol	1555.00		NIST Webbook
tb	649.20	K	Joback Method
tc	848.77	K	Joback Method
tf	379.39	K	Joback Method
vc	0.733	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	577.68	J/mol×K	649.20	Joback Method
cpg	596.22	J/mol×K	682.46	Joback Method
cpg	613.82	J/mol×K	715.72	Joback Method
cpg	630.63	J/mol×K	748.99	Joback Method
cpg	646.79	J/mol×K	782.25	Joback Method
cpg	662.43	J/mol×K	815.51	Joback Method
cpg	677.71	J/mol×K	848.77	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=R232892&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

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