Ischwarone

Inchi: InChI=1S/C15H22O/c1-9-4-5-12(16)15-7-11-10(6-14(9,15)3)13(11,2)8-15/h9-11H,4-8H2,
InchiKey: FADPMTSJYFTYLF-KDBIFJDOSA-N
Formula: C15H22O
SMILES: CC1CCC(=O)C23CC4C(CC12C)C4(C)C3
Mol. weight [g/mol]: 218.33

Physical Properties

Property code	Value	Unit	Source
gf	163.94	kJ/mol	Joback Method
hf	-194.39	kJ/mol	Joback Method
hfus	9.90	kJ/mol	Joback Method
hvap	48.81	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	3.428		Crippen Method
mcvol	180.340	ml/mol	McGowan Method
pc	2417.12	kPa	Joback Method
rinpol	1682.00		NIST Webbook
tb	628.76	K	Joback Method
tc	874.39	K	Joback Method
tf	462.01	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	543.64	J/mol×K	628.76	Joback Method
cpg	565.38	J/mol×K	669.70	Joback Method
cpg	586.03	J/mol×K	710.64	Joback Method
cpg	606.12	J/mol×K	751.57	Joback Method
cpg	626.18	J/mol×K	792.51	Joback Method
cpg	646.74	J/mol×K	833.45	Joback Method
cpg	668.32	J/mol×K	874.39	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R587390&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume