(3S,4aR,5S,8aS)-4a,5-Dimethyl-3-(prop-1-en-2-yl)-2

Inchi: InChI=1S/C15H22O/c1-10(2)12-8-14(16)13-7-5-6-11(3)15(13,4)9-12/h5,7,11-13H,1,6,8-9
InchiKey: CSROQEWHHKSXKD-UHFFFAOYSA-N
Formula: C15H22O
SMILES: C=C(C)C1CC(=O)C2C=CCC(C)C2(C)C1
Mol. weight [g/mol]: 218.33
CAS: 22489-11-8

Physical Properties

Property code	Value	Unit	Source
gf	114.27	kJ/mol	Joback Method
hf	-221.69	kJ/mol	Joback Method
hfus	16.46	kJ/mol	Joback Method
hvap	51.68	kJ/mol	Joback Method
log10ws	-3.91		Crippen Method
logp	3.760		Crippen Method
mcvol	193.460	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1694.10		NIST Webbook
rinpol	1694.10		NIST Webbook
tb	627.60	K	Joback Method
tc	864.65	K	Joback Method
tf	349.29	K	Joback Method
vc	0.729	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.43	J/mol×K	627.60	Joback Method
cpg	564.57	J/mol×K	667.11	Joback Method
cpg	586.34	J/mol×K	706.62	Joback Method
cpg	606.88	J/mol×K	746.12	Joback Method
cpg	626.34	J/mol×K	785.63	Joback Method
cpg	644.87	J/mol×K	825.14	Joback Method
cpg	662.61	J/mol×K	864.65	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22489118&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