(E)-3-((5R,7R,7aR)-3,7-Dimethyl-2,4,5,6,7,7a-hexah

Inchi: InChI=1S/C15H24O/c1-10(9-16)6-13-7-12(3)14-5-4-11(2)15(14)8-13/h6,12-14,16H,4-5,7
InchiKey: WDYKMPVPVCJTKA-GHKOFPOXSA-N
Formula: C15H24O
SMILES: CC(=CC1CC2=C(C)CCC2C(C)C1)CO
Mol. weight [g/mol]: 220.35
CAS: 1372763-27-3

Physical Properties

Property code	Value	Unit	Source
gf	98.46	kJ/mol	Joback Method
hf	-256.11	kJ/mol	Joback Method
hfus	29.07	kJ/mol	Joback Method
hvap	67.35	kJ/mol	Joback Method
log10ws	-4.14		Crippen Method
logp	3.698		Crippen Method
mcvol	197.760	ml/mol	McGowan Method
pc	2064.24	kPa	Joback Method
rinpol	1704.20		NIST Webbook
rinpol	1680.40		NIST Webbook
tb	669.56	K	Joback Method
tc	870.07	K	Joback Method
tf	347.47	K	Joback Method
vc	0.750	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.51	J/mol×K	669.56	Joback Method
cpg	592.58	J/mol×K	702.98	Joback Method
cpg	609.62	J/mol×K	736.40	Joback Method
cpg	625.71	J/mol×K	769.82	Joback Method
cpg	640.89	J/mol×K	803.24	Joback Method
cpg	655.23	J/mol×K	836.66	Joback Method
cpg	668.78	J/mol×K	870.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1372763273&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