

(1aR,4aS,8aS)-4a,8,8-Trimethyl-1,1a,4,4a,5,6,7,8-o

Inchi:	InChI=1S/C15H22O/c1-13(2)6-4-7-14(3)8-5-11(10-16)12-9-15(12,13)14/h5,10,12H,4,6-9
InchiKey:	CLNRASCYJGCDIN-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC1(C)CCCC2(C)CC=C(C=O)C3CC312
Mol. weight [g/mol]:	218.33
CAS:	470-41-7

Physical Properties

Property code	Value	Unit	Source
gf	130.10	kJ/mol	Joback Method
hf	-160.74	kJ/mol	Joback Method
hfus	10.11	kJ/mol	Joback Method
hvap	52.98	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2448.32	kPa	Joback Method
rinpol	1724.20		NIST Webbook
tb	620.21	K	Joback Method
tc	856.90	K	Joback Method
tf	428.33	K	Joback Method
vc	0.727	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	526.78	J/molxK	620.21	Joback Method
cpg	546.55	J/molxK	659.66	Joback Method
cpg	565.25	J/molxK	699.11	Joback Method
cpg	583.33	J/molxK	738.56	Joback Method
cpg	601.25	J/molxK	778.01	Joback Method
cpg	619.48	J/molxK	817.45	Joback Method
cpg	638.48	J/molxK	856.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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=C470417&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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