(1aS,4aS,8aR)-4a,8,8-Trimethyl-2-methylene-1,1a,2

Inchi: InChI=1S/C15H22/c1-11-6-9-14(4)8-5-7-13(2,3)15(14)10-12(11)15/h6,9,12H,1,5,7-8,10H
InchiKey: XOPQCMQCJQEISN-UHFFFAOYSA-N
Formula: C15H22
SMILES: C=C1C=CC2(C)CCCC(C)(C)C23CC13
Mol. weight [g/mol]: 202.34
CAS: 51446-91-4

Physical Properties

Property code	Value	Unit	Source
gf	292.33	kJ/mol	Joback Method
hf	20.55	kJ/mol	Joback Method
hfus	7.05	kJ/mol	Joback Method
hvap	45.76	kJ/mol	Joback Method
log10ws	-4.53		Crippen Method
logp	4.335		Crippen Method
mcvol	181.030	ml/mol	McGowan Method
pc	2354.20	kPa	Joback Method
rinpol	1471.70		NIST Webbook
rinpol	1471.70		NIST Webbook
tb	565.73	K	Joback Method
tc	801.71	K	Joback Method
tf	387.49	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	480.56	J/mol×K	565.73	Joback Method
cpg	501.99	J/mol×K	605.06	Joback Method
cpg	521.76	J/mol×K	644.39	Joback Method
cpg	540.33	J/mol×K	683.72	Joback Method
cpg	558.16	J/mol×K	723.05	Joback Method
cpg	575.70	J/mol×K	762.38	Joback Method
cpg	593.40	J/mol×K	801.71	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=C51446914&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