

Neoisolongifolene, 8-oxo-

Other names:	8-oxo-neoisolongifolene
Inchi:	InChI=1S/C15H22O/c1-13(2)7-6-12(16)15-8-5-10(9-11(13)15)14(15,3)4/h9-10H,5-8H2,1
InchiKey:	OAUCHXPHYIWYEW-UHFFFAOYSA-N
Formula:	C15H22O
SMILES:	CC1(C)CCC(=O)C23CCC(C=C12)C3(C)C
Mol. weight [g/mol]:	218.33

Physical Properties

Property code	Value	Unit	Source
gf	107.03	kJ/mol	Joback Method
hf	-212.86	kJ/mol	Joback Method
hfus	7.33	kJ/mol	Joback Method
hvap	50.51	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.738		Crippen Method
mcvol	186.900	ml/mol	McGowan Method
pc	2356.49	kPa	Joback Method
rinpol	1808.00		NIST Webbook
tb	639.37	K	Joback Method
tc	887.45	K	Joback Method
tf	454.55	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.19	J/molxK	639.37	Joback Method
cpg	559.31	J/molxK	680.72	Joback Method
cpg	579.56	J/molxK	722.06	Joback Method
cpg	599.42	J/molxK	763.41	Joback Method
cpg	619.37	J/molxK	804.76	Joback Method
cpg	639.89	J/molxK	846.10	Joback Method
cpg	661.47	J/molxK	887.45	Joback Method

Sources

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=U152033&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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