Neoisolongifolene, 8-bromo-

Inchi: InChI=1S/C15H23Br/c1-13(2)7-6-12(16)15-8-5-10(9-11(13)15)14(15,3)4/h9-10,12H,5-8H
InchiKey: DRISYGHYCMWXSH-UHFFFAOYSA-N
Formula: C15H23Br
SMILES: CC1(C)CCC(Br)C23CCC(C=C12)C3(C)C
Mol. weight [g/mol]: 283.25

Physical Properties

Property code	Value	Unit	Source
gf	236.23	kJ/mol	Joback Method
hf	-69.17	kJ/mol	Joback Method
hfus	14.18	kJ/mol	Joback Method
hvap	52.38	kJ/mol	Joback Method
log10ws	-5.22		Crippen Method
logp	4.933		Crippen Method
mcvol	202.830	ml/mol	McGowan Method
pc	2358.78	kPa	Joback Method
rinpol	1639.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	633.04	K	Joback Method
tc	880.87	K	Joback Method
tf	441.89	K	Joback Method
vc	0.770	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	552.46	J/mol×K	633.04	Joback Method
cpg	573.44	J/mol×K	674.35	Joback Method
cpg	593.40	J/mol×K	715.65	Joback Method
cpg	612.87	J/mol×K	756.96	Joback Method
cpg	632.40	J/mol×K	798.26	Joback Method
cpg	652.51	J/mol×K	839.57	Joback Method
cpg	673.73	J/mol×K	880.87	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U151648&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
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