(1S,5S)-2-Methyl-5-((R)-6-methylhept-5-en-2-yl)bic

Other names: 7-epi-Sesquithujene
Episesquithujene
Inchi: InChI=1S/C15H24/c1-11(2)6-5-7-13(4)15-9-8-12(3)14(15)10-15/h6,8,13-14H,5,7,9-10H2,
InchiKey: UCQHFDKBUHCAFR-KKUMJFAQSA-N
Formula: C15H24
SMILES: CC(C)=CCCC(C)C12CC=C(C)C1C2
Mol. weight [g/mol]: 204.35
CAS: 159407-35-9

Physical Properties

Property code	Value	Unit	Source
gf	280.99	kJ/mol	Joback Method
hf	-43.63	kJ/mol	Joback Method
hfus	20.78	kJ/mol	Joback Method
hvap	48.26	kJ/mol	Joback Method
log10ws	-4.87		Crippen Method
logp	4.725		Crippen Method
mcvol	191.890	ml/mol	McGowan Method
pc	1945.79	kPa	Joback Method
rinpol	1408.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1391.00		NIST Webbook
tb	564.06	K	Joback Method
tc	768.86	K	Joback Method
tf	297.83	K	Joback Method
vc	0.749	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	495.08	J/mol×K	564.06	Joback Method
cpg	514.58	J/mol×K	598.19	Joback Method
cpg	532.84	J/mol×K	632.33	Joback Method

cpg	550.02	J/mol×K	666.46	Joback Method
cpg	566.29	J/mol×K	700.59	Joback Method
cpg	581.82	J/mol×K	734.73	Joback Method
cpg	596.76	J/mol×K	768.86	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=C159407359&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