7-epi-Sesquithujene

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

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	1391.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1387.00		NIST Webbook
rinpol	1406.00		NIST Webbook
rinpol	1391.00		NIST Webbook
rinpol	1386.00		NIST Webbook
rinpol	1393.00		NIST Webbook
rinpol	1406.00		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=R610569&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