«gamma»-Neoclovene

Inchi: InChI=1S/C15H24/c1-11-6-5-8-14(4)12-7-9-15(11,14)10-13(12,2)3/h5-6,11-12H,7-10H2,1
InchiKey: ZYKFQRCKKGFKQR-UHFFFAOYSA-N
Formula: C15H24
SMILES: CC1C=CCC2(C)C3CCC12CC3(C)C
Mol. weight [g/mol]: 204.35

Physical Properties

Property code	Value	Unit	Source
gf	231.54	kJ/mol	Joback Method
hf	-84.03	kJ/mol	Joback Method
hfus	9.28	kJ/mol	Joback Method
hvap	45.29	kJ/mol	Joback Method
log10ws	-4.43		Crippen Method
logp	4.415		Crippen Method
mcvol	185.330	ml/mol	McGowan Method
pc	2239.76	kPa	Joback Method
ripol	1754.00		NIST Webbook
tb	561.90	K	Joback Method
tc	795.76	K	Joback Method
tf	369.57	K	Joback Method
vc	0.709	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	501.64	J/mol×K	561.90	Joback Method
cpg	524.98	J/mol×K	600.88	Joback Method
cpg	546.53	J/mol×K	639.85	Joback Method
cpg	566.74	J/mol×K	678.83	Joback Method
cpg	586.06	J/mol×K	717.81	Joback Method
cpg	604.93	J/mol×K	756.78	Joback Method
cpg	623.79	J/mol×K	795.76	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=U156117&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume